

12. Semiconductor Fundamentals

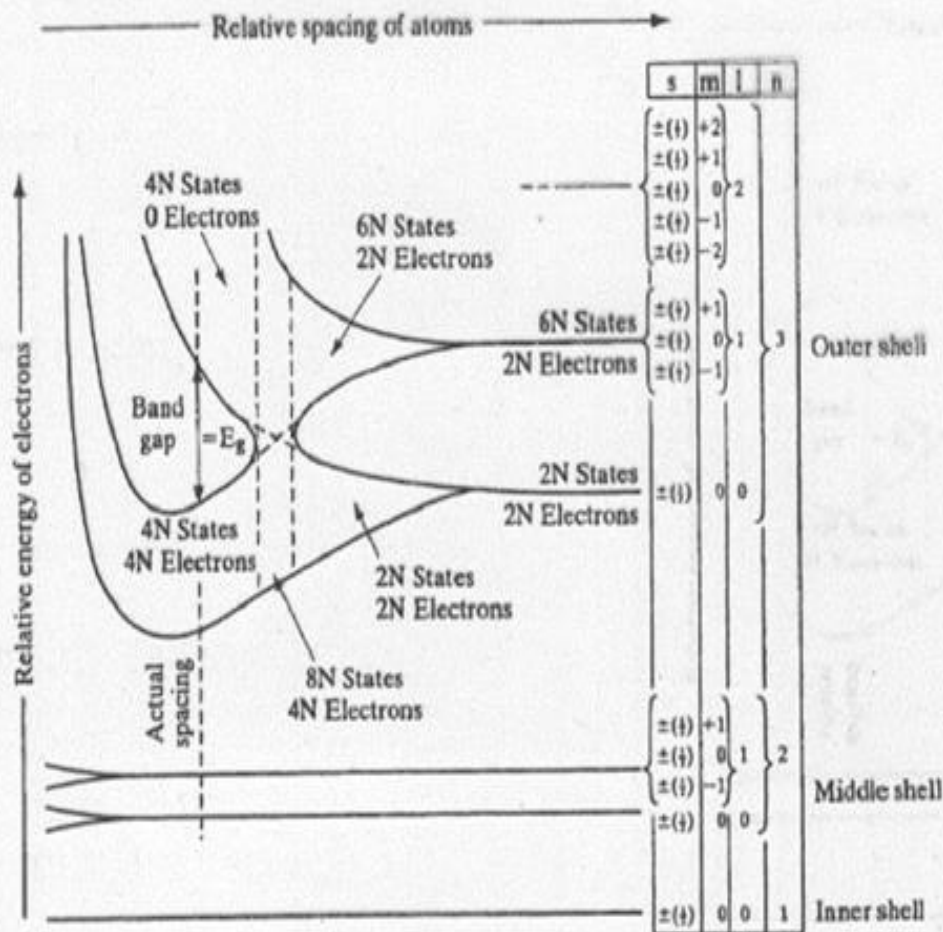


Figure 3-3

Energy levels in Si as a function of inter-atomic spacing. The core levels ($n = 1, 2$) in Si are completely filled with electrons. At the actual atomic spacing of the crystal, the $2N$ electrons in the $3s$ sub-shell and the $2N$ electrons in the $3p$ sub-shell undergo sp^3 hybridization, and all end up in the lower $4N$ states (valence band), while the higher lying $4N$ states (conduction band) are empty, separated by a bandgap.

- Si : IC

(Memory & logic circuits, Analysis, Amplifiers, power devices)

- GaAs : Alternative to Si in some special systems

(Microwave, Optoelectronics, High-speed devices)

1-1 Crystal structure

1) Solids : crystalline, polycrystalline, amorphous

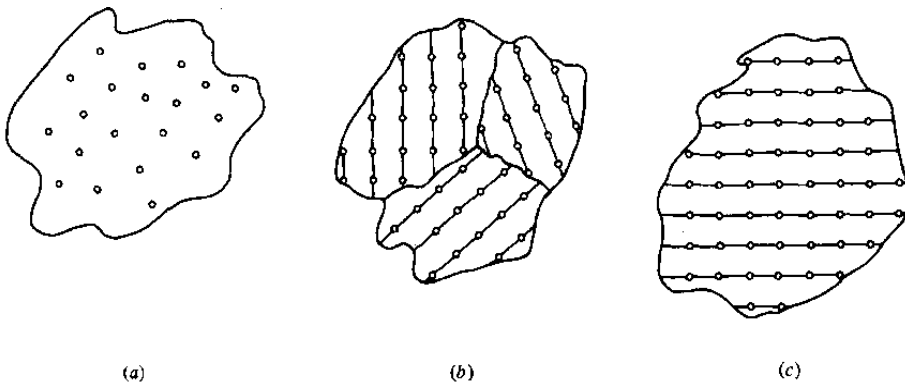


FIGURE 1-1

Three classes of solids: (a) amorphous, (b) polycrystalline, and (c) crystalline.

① Amorphous solid (Fig 1-1 a)

(not well-defined structure, formlessness)

- a-Si

[low-cost solar cells : calculators
a-FETs : large-area displays, image sensors

- a-SiO₂ : extremely important material in S/C technology
→ insulator

② Polycrystalline solid (Fig 1-1 b)

many small regions, each region

- has a well organized structure but differs from its neighboring regions
 - can be produced inexpensively
 - be used extensively in microelectronics
- ex) poly-Si : conductor, contact, gate in transistors

③ Crystalline solid (Fig 1-1 c)

atoms are arranged in an orderly array

→ periodic structure (=lattice)

- unit cell → repeat ⇒ crystalline solid

2) Five cubic structures

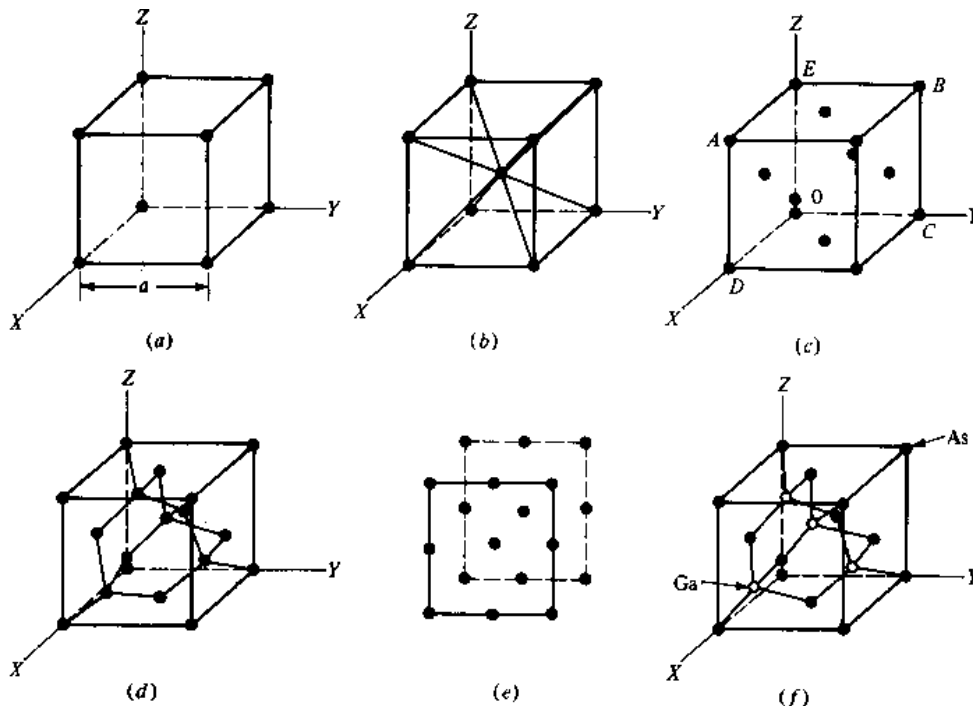


FIGURE 1-3

Unit cells of cubic crystals: (a) simple cubic, (b) body-centered cubic, (c) face-centered cubic, (d) diamond, (e) two penetrating fcc lattices in two dimensions, (f) zinc blende.

① sc crystal (Fig 1-3 a)

- each corner of the cubic lattice is occupied by an atom
- each atom is shared by eight neighboring unit cells
- dimension “a” = lattice constant

ex) Po (polonium)

② bcc crystal (Fig 1-3 b)

- an atoms is located at the center of the cubic

ex) Na, Mo, W

③ fcc crystal (Fig 1-3 c)

- each atom is located at each of the six cubic faces

ex) Al, Cu, Au, Ni, Pt

④ Diamond structure (Fig 1-3 d)

- two interpenetrating fcc sublattices with one displaced from the other by $\frac{1}{4}$ of the distance along a diagonal of the cubic
- Fig 1-3 e : top view

→ 4 atoms belong to the first fcc lattice

ex) Si, Ge

⑤ Zinc blende structure (Fig 1-3 f)

- two different atoms (GaAs)

Ga atoms are placed on one fcc lattice

As atoms are placed on the other fcc lattice

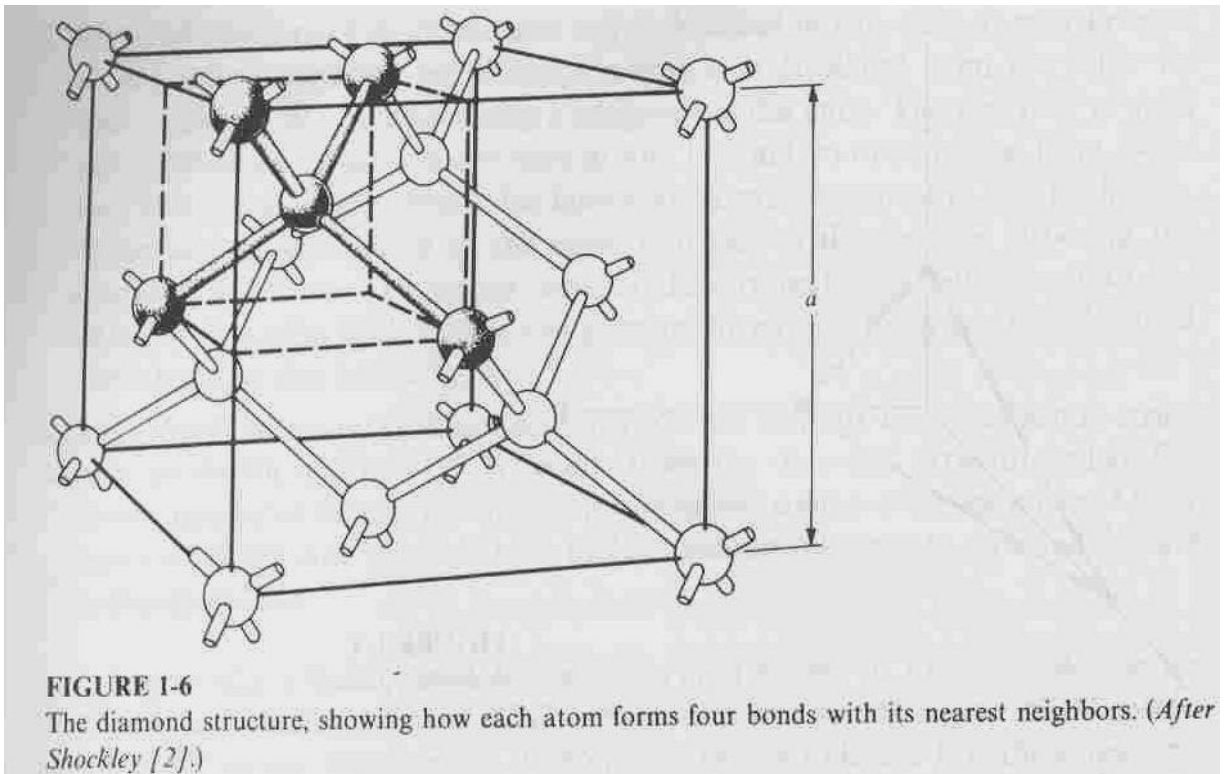
ex) GaAs, GaP, ZnS, CdS

3) Consider fcc crystal (Fig 1-3 c)

- ABCD place : 6 atoms
 - AEOD place : 5 atoms
- } Atomic spacing are different

→ Crystal properties along different directions are different
(=crystal is anisotropic)

4) Consider diamond structure (Fig 1-6)



- each atom bonds with its 4 nearest neighbors
→ form a tetrahedron
- tetrahedral bond
very strong, directional → give rise to specific mechanical,

metallurgical, and electrical properties of the solid.

- In GaAs, tetrahedral bond between Ga and As
- Tetrahedral configuration → specifies the bond angles and lengths with a perfect symmetry
- If the bond angles change more than 10° , Si will be amorphous

※ What is the bonding force between the two neighboring atoms?

1-2 Bohr's Atom

1) The simplest model of an atom :

a positively charged nucleus with negatively charged electrons orbiting around it.

① Bohr : angular momentum of an electron has certain discrete values $\rightarrow$ give rise to a set of discrete allowable energy levels

- For hydrogen atom

$$E_n = -\frac{13.6}{n^2} \text{ eV}$$

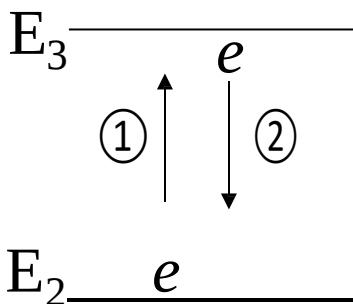
n : principal Q. N.

E_n : electron binding energy

E_1 : -13.6 eV $\rightarrow$ lowest energy level $\Rightarrow$ ground state

E_2 : -3.41 eV
 E_3 : -1.53 eV
 E_4 : ...

} excited state



① : electron must gain energy, $E_3 - E_2$

② : electron must emit energy, $E_3 - E_2$
 quantum of energy
 = light (photon)

- For the transition between E_2 and E_1

$$E_2 - E_1 = h\nu$$

h : planck's constant

ν : frequency of the absorbed or emitted energy
corresponding wavelength

$$\lambda = \frac{c}{\nu} \quad (c : \text{velocity of light})$$

2) Filling of electrons

- ① For an atom with electrons more than one, the lowest energy level is the first to be filled, followed by the filling up of each successively higher energy level

$n = 1 \rightarrow \text{K - shell} \rightarrow E_1 \text{ has 2 energy states} \rightarrow 2 \text{ electrons}$

$n = 2 \rightarrow \text{L - shell} \rightarrow E_2 \text{ has 8 energy states} \rightarrow 8 \text{ electrons}$

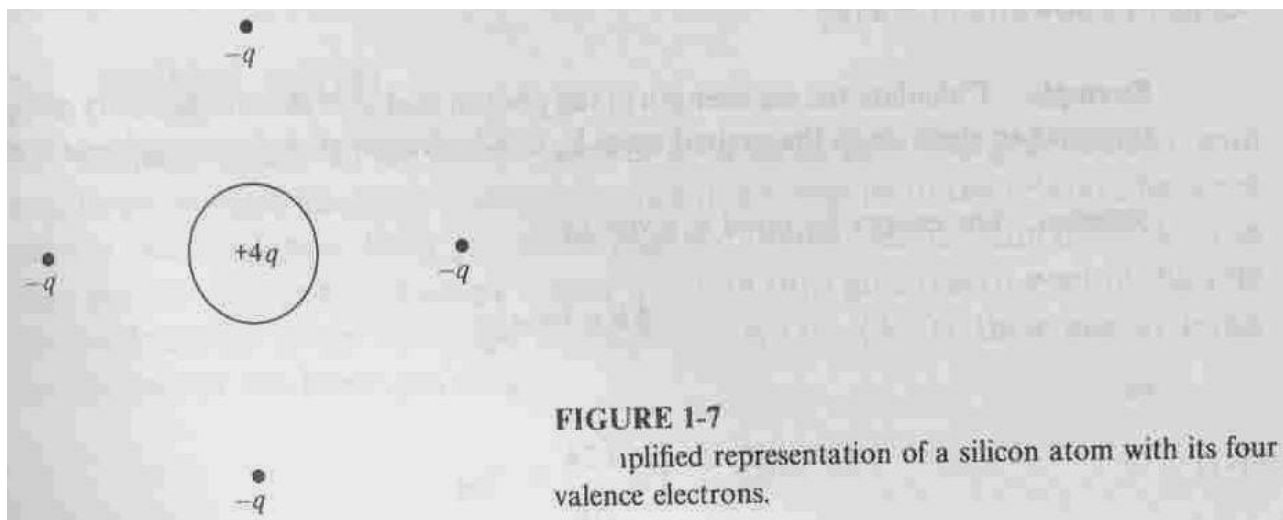
$n = 3 \rightarrow \text{M - shell} \rightarrow E_3 \text{ has 18 energy states} \rightarrow 18 \text{ electrons}$

$\rightarrow \text{Distribution of electrons} \Rightarrow \text{"chemical properties"}$

- ② For an isolated Si atom,

14 electrons $\left\{ \begin{array}{l} 2 \text{ in K - shell}(E_1) \\ 8 \text{ in L - shell}(E_2) \end{array} \right\} \text{ tightly bound electrons (TBE)}$
 $\left\{ \begin{array}{l} 4 \text{ in M - shell}(E_3) \end{array} \right\} \text{ - valence electrons(VE)}$

- $\left\{ \begin{array}{l} \text{TBE : do not participate in chemical reaction or interatomic bonding} \\ \text{VE : participate in chemical reaction or interatomic bonding} \end{array} \right.$



1-3 Valence-band Model of Solid

① In a crystal lattice,

a positively charged nucleus is surrounded by negatively charged orbiting electrons in each constituent atom.

- If the atoms are closely packed, the orbits of the outer-shell electrons will overlap to produce strong interatomic forces
- The outer electrons(valence electrons) determine the electrical properties of the solid!
- Metallic conductors(Al, Au etc) – valence electrons are free to move and are not bound to individual atoms.

→ When an electric field is applied, valence electrons move

→ “current flow”

{ free electron density $\sim 10^{23} / \text{cm}^3$
resistivity $\sim 10^{-5} \Omega \cdot \text{cm}$

- Insulators (quartz(SiO_2)) – almost all the valence electrons are bond to the constituent atoms

→ can not flow current

resistivity $\sim 10^{16} \Omega \cdot \text{cm}$

- Crystalline semiconductor (Si) – each atom has 4 VEs to share with its four nearest-neighboring atoms.

→ forms “covalent bond”

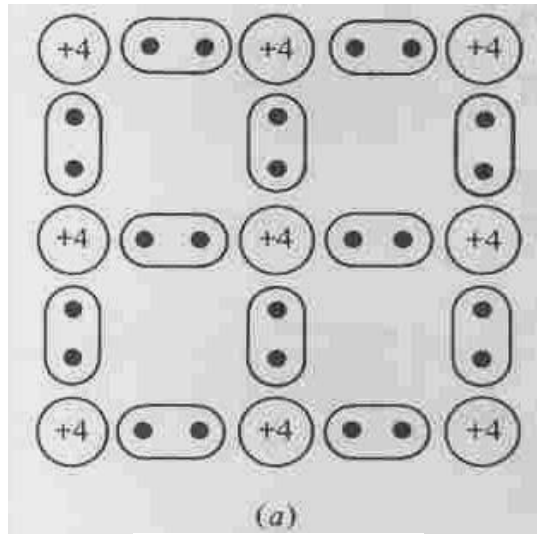


Fig. 1-8 (a)

- At low T, electrons are bound and not available for conduction
- At high T, thermal E enables some electrons to break the bond, and the liberated electrons are then free to contribute to current conduction

→ A semiconductor behaves like an insulator at low T and a conductor at high T

cf) at room temperature, ρ of pure Si $\sim 2 \times 10^5 \Omega \cdot \text{cm}$
(considerably higher than that of a good conductor)

- ② When a valence electron is liberated in a semiconductor, a vacancy is left behind in the covalent bond.

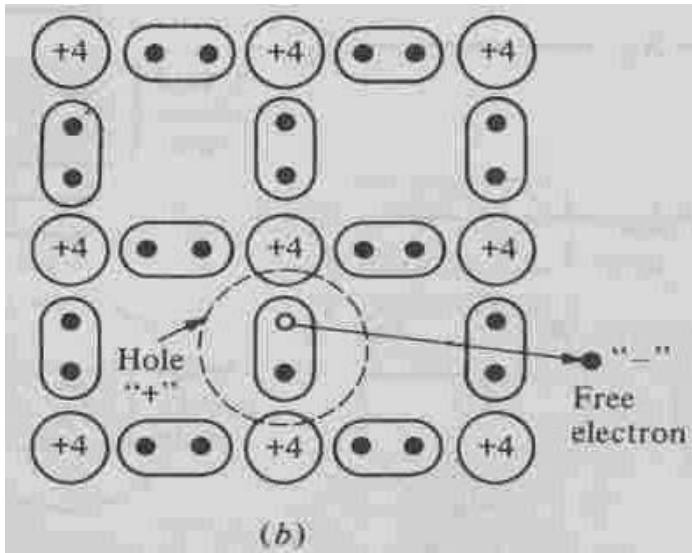
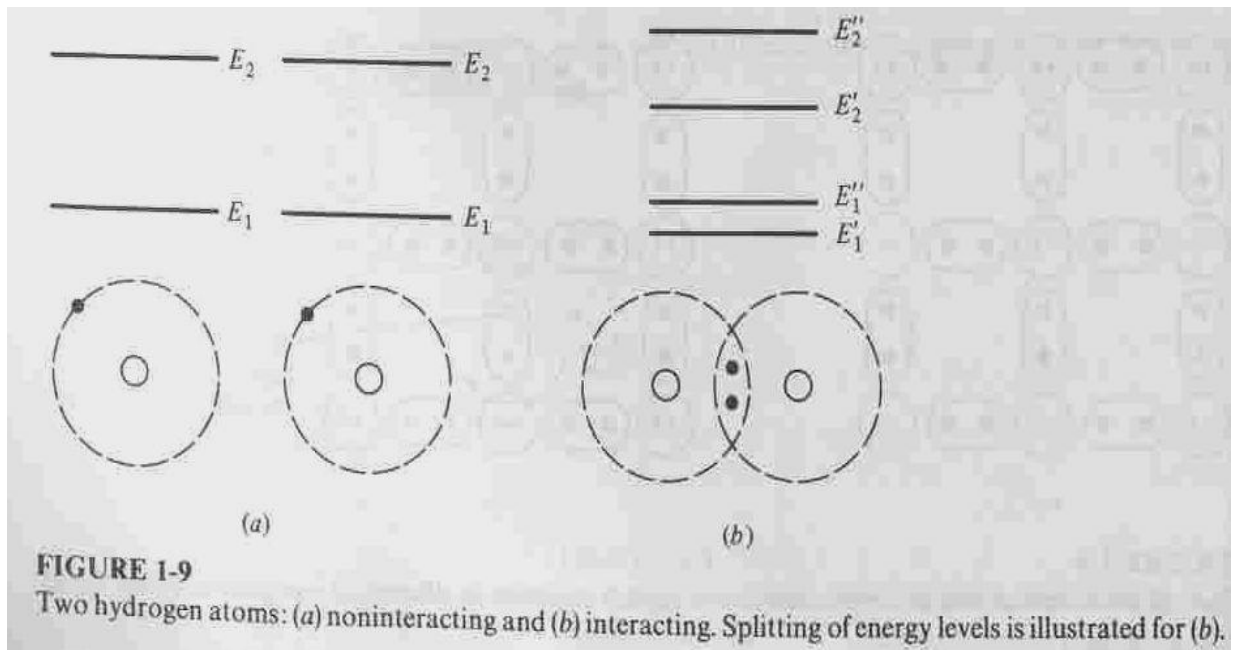


Fig 1-8 (b)

- This vacancy may be filled by one of its neighboring valence electrons → result in a shift of the vacancy location.
→ vacancy moves inside the crystalline structure.
- ➡ This vacancy may be considered as a particle analogous to an electron
- ➡ “Fictitious particle” = “hole”
→ carries a positive charge and moves in the direction opposite that of an electron under an externally applied electric field

1-4 Energy-band Model of Solid

- ① In Sec. 1-2, only isolated atom has been considered, and the theory is applicable to element in the gaseous state in which individual atoms are widely separated.
- ② In solid, the atoms are closely packed, and they tend to interact.



- Individual atoms have identical energy states
- When the two hydrogen atoms become close to form molecular hydrogen, the electron orbits start to overlap
→ each energy level splits into two discrete levels
- In a solid, the atomic interaction involves more than two atoms
→ electrons in the out most shell are shared by many atoms
➡ each energy level will split into a band of energy

※ Atomic spacing of the atoms affects the nature of the separation of bands and their properties
(if we can adjust the atomic spacing of a material, we can control its energy band!)

③ Electrons are allowed to reside within the energy bands but not between the bands of allowed energy states

→ there is gaps of forbidden energies in which an electron cannot exist.

- Each allowed energy band contains a limited number of states that can accommodate a definite number of electrons

- In a semiconductor, the valence electrons group together to occupy a band of energy levels

= valence band

- the next higher band of allowed energy levels (=conduction band)

is separated from the forbidden gap of energy, E_g

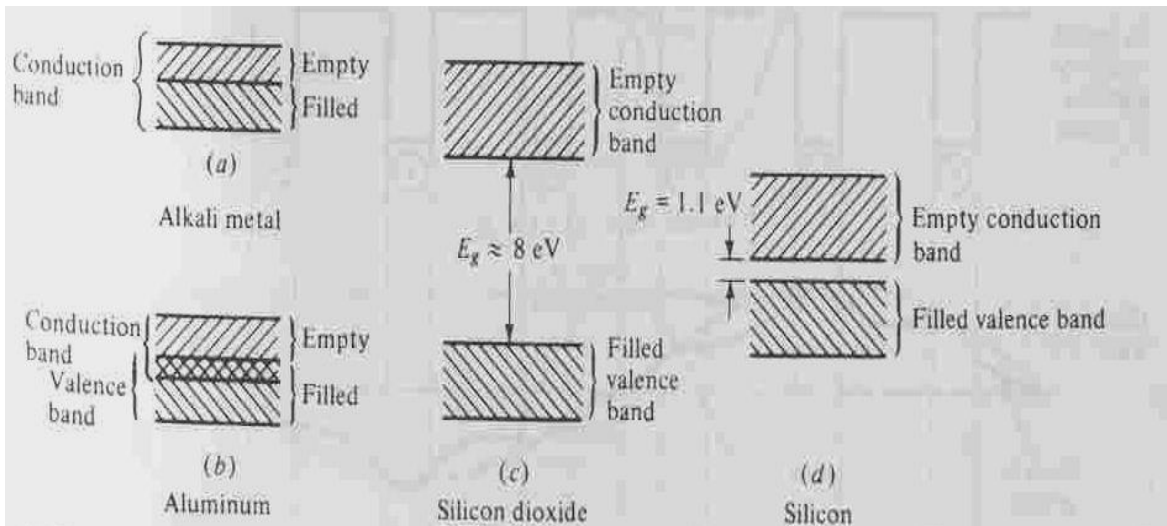


FIGURE 1-10

Energy-band diagrams for (a and b) metals, (c) insulator, and (d) semiconductor at 0 K. The vertical axis represents the energy, and the horizontal axis represents spatial position.

- For metals, conduction band is only partially filled by electrons (Alkali metal, (a)) or two bands are overlapped so that there is no forbidden gap (Al, (b))
- For insulators, valence band is completely filled and conduction band is empty (c) → No current flows
 - Energy should be added for electrons in the filled V.B. to jump to the C.B.
 - However, E_g in insulator is too large to jump ($E_g > 5 \text{ eV}$)
- In semiconductor, E_g is not too large (d)
 - ex) $E_g = 1.12 \text{ eV}$ (Si), 1.43 eV (GaAs)
 - corresponds to the not-so-tight bonding of the valence electrons

- ④ At R.T., some electrons in V.B. may receive enough thermal Energy to overcome the E_g and reach C.B.

→ electrons in C.B.
holes in V.B. } → Under applied external electric field,
current flows

∴ Electrical conduction in a semiconductor may take place by two distinct and independent mechanism

$$I_{\text{tot}} = \underbrace{I_e}_{\text{in C.B.}} + \underbrace{I_h}_{\text{in V.B.}}$$

1.5 The concepts of effective mass

- ① electrons carry a charge $-q$
holes carry a charge $+q$

- ② Each particles carries a mass
 $\neq$ electron mass m_e in free space

- ③ The mass of a carrier depends on

{

the energy band it occupies
the momentum of the carrier
the direction of the applied field

④ In most cases, the masses of the carriers are lighter than m_0
(= they behave differently from the classical particles)

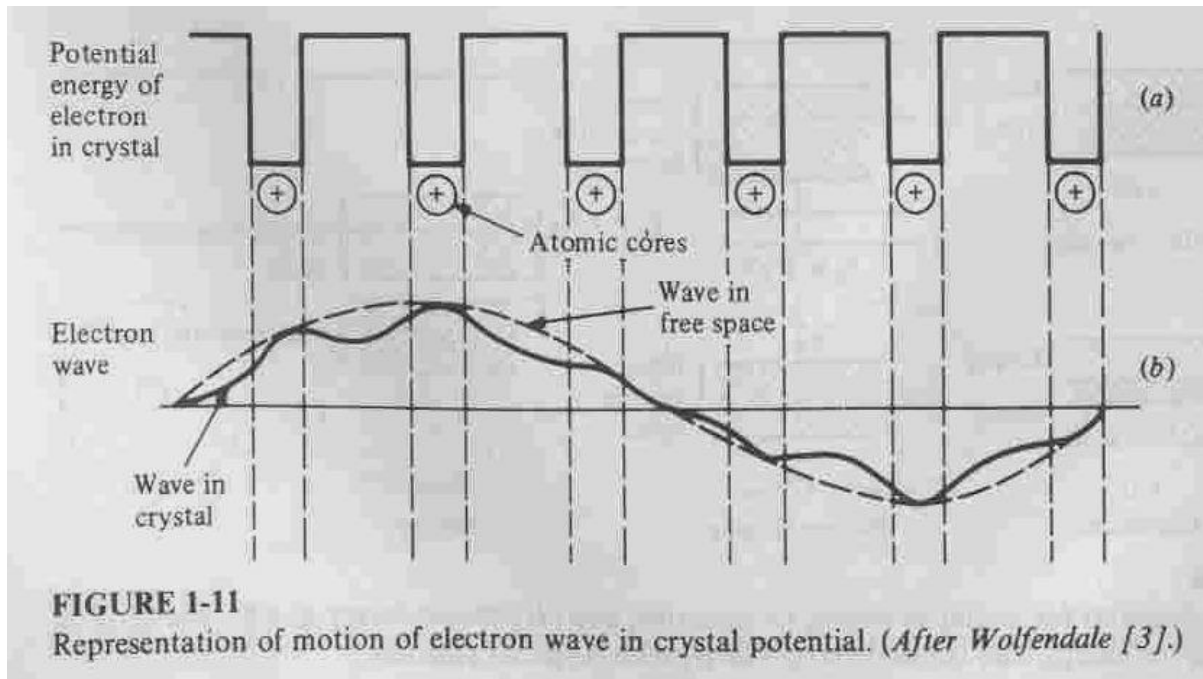
⑤ In Q.M., an electron is a traveling wave with a wavelength
and a crystal momentum P

➡ de Broglie relation

$$P = \frac{h}{\lambda} = \frac{hk}{2\pi} = \hbar k$$

$k = 2\pi/\lambda$ and called “wave number”

- An electron in a one-D lattice at 0 k



- ① Potential E of electron decreases as the electron passes by the positively charged atomic core
- ② The electron wave in free space is a pure sinusoid (dashed curve), but it is distributed in the solid by the crystal's periodic potential(solid curve)
- ③ The amplitude of the electron wave increases slightly in the neighborhood of the atomic cores ($\because$ coulombic attraction), but the electron propagates freely in spite of the interference
 → the difference between the solid and dashed curves illustrates that the mass of the electron in a solid is different from the

electron mass in free space $\Rightarrow$ effective mass

- ④ consider the electron in a solid as a classical particle, having the energy – momentum relationship

$$E = \frac{p^2}{2m_e} = \frac{h^2 k^2}{8\pi^2 m_e}$$

E = kinetic energy

- ⑤ from quantum mechanical consideration,

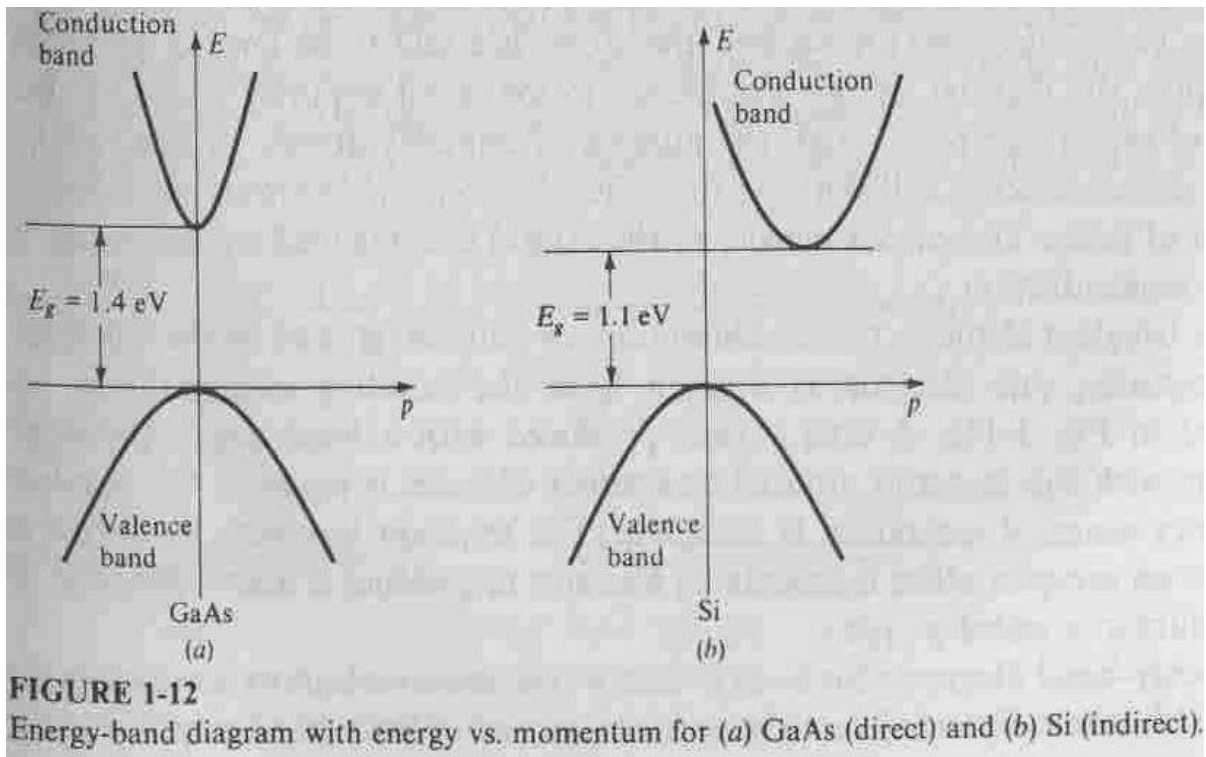
$$m_e = \frac{h^2 / 4\pi^2}{\partial^2 E / \partial k^2} \quad \text{----- (1-6)}$$

→ effective mass can be calculated if E – k relationship is known

“ $\partial^2 E / \partial k^2$ = curvature of E – k curve ”

- ⑥ more complicated energy – band diagrams

(the top of the valence band is taken as the reference level)



- GaAs : the lowest C.B minimum is located at zero momentum
(=directly above the V.B minimum)
→ direct band-gap semiconductor
- Si : the lowest C.B minimum is not at zero momentum
→ indirect band-gap semiconductor

cf) In either crystal, E_g = the difference between the lowest C.B. minimum and the V.B. maximum

- Using Eq. (1-6), it is possible to derive m_e for electrons in C.B. and holes in V.B.

(sharper C.B. of GaAs → large curvature → small m_e for its electrons)

1-6 Intrinsic & Extrinsic S/Cs

- In a perfect S/C, $n=p$

($\because$ the process of producing an electron in the CB creates a hole in the VB)

➡ “Intrinsic S/C”

$$n = p = n_i \quad (1-7)$$

n_i : intrinsic carrier conc.

cf) n_i in most S/C is very low $\rightarrow$ not usable for device purposes

- In practical devices, the carrier concentration is controlled by adding impurity (= doping)
= dopant

➡ “doped S/C” = “Extrinsic S/C”

1) Si : Group V elements (P, As, Sb etc)

$\rightarrow$ each substitutional atom supplies 5 electrons

$\rightarrow$ one extra electron that is necessary for making the covalent bonds.

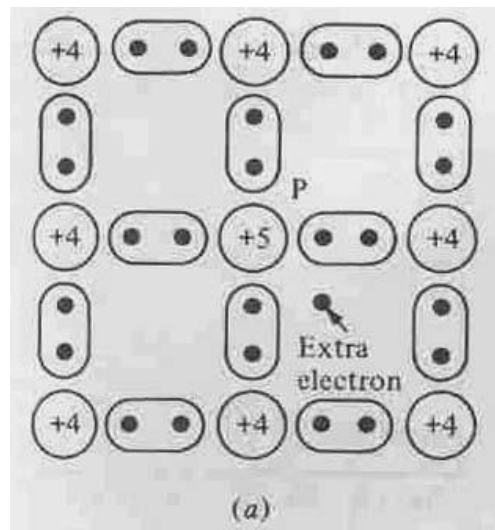


FIGURE 1-13

Crystal structure of silicon with a silicon atom displaced by (a) a pentavalent (donor) impurity atom and (b) a trivalent (acceptor) impurity atom.

- Excess electron is rather loosely bound to atom and can easily be set free.
- Each atom donates an excess electron in Si $\Rightarrow$ “Donor”
- Free electrons carry a negative charge and leave behind a fixed positive charge with the impurity atoms $\rightarrow$ “charge – neutrality condition” is preserved
- $\Rightarrow$ No vacancy in the lattice site to produce a hole!
- When the excess electrons are set free, the atoms are said to be ionized
- If the thermal E is sufficient to ionize all impurity atoms, the No. of excess electrons equals the No. of impurity atoms.
- Call it “n-type S/C ($n \gg p$)”
- The carrier density of the crystal is controlled by the group **V** impurity concentration

2) Si : Group III elements (B, Al, Ga etc)

→ one electron is missing from the covalent bonds

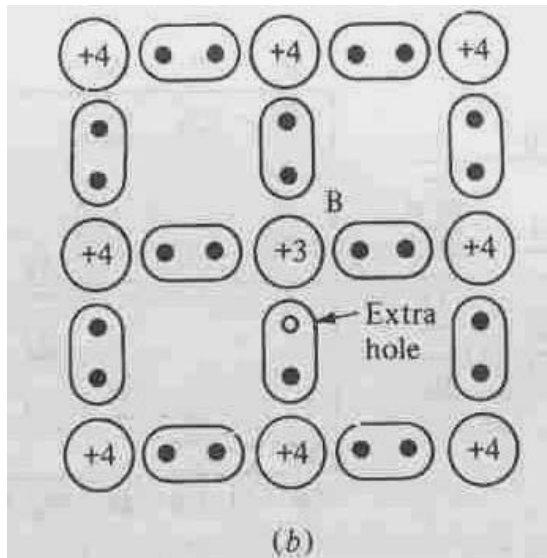


FIGURE 1-13

Crystal structure of silicon with a silicon atom displaced by (a) a pentavalent (donor) impurity atom and (b) a trivalent (acceptor) impurity atom.

- A hole is produced with a fixed negative charge remaining with the impurity atom

- Call this impurity in Si ⇒ “ acceptor ”

(∵ it accepts an electron to produce a hole)

⇒ “ p-type S/C “ ($p \gg n$)

3) Energy-band diagram

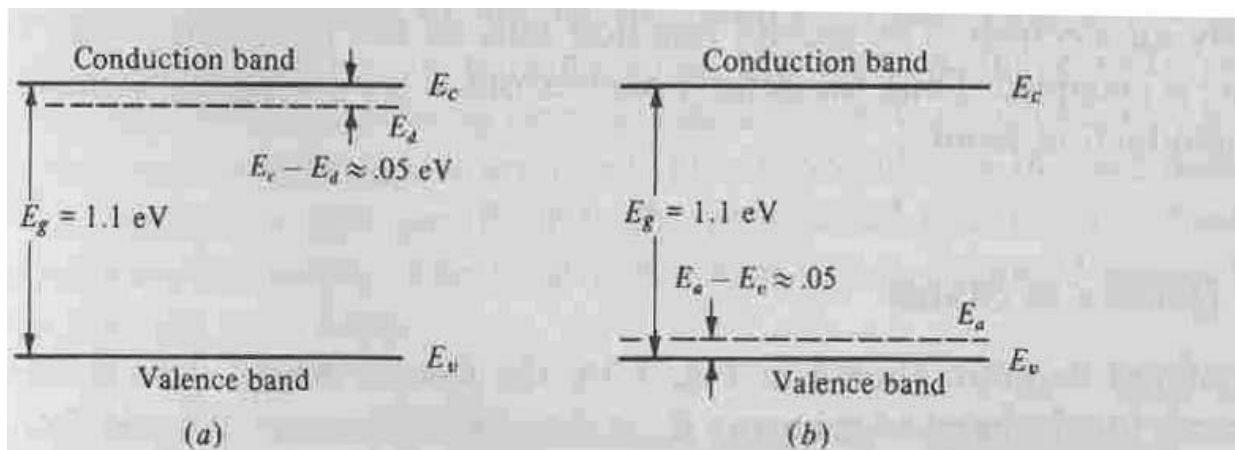


FIGURE 1-14

Energy-band diagram of (a) an *n*-type semiconductor and (b) a *p*-type semiconductor.

E_a = acceptor energy level

$E_a - E_v$ = ionization energy of the acceptor impurity

E_d = donor energy level

$E_c - E_d$ = ionization energy of the donor impurity

• Ionization energies of some impurities

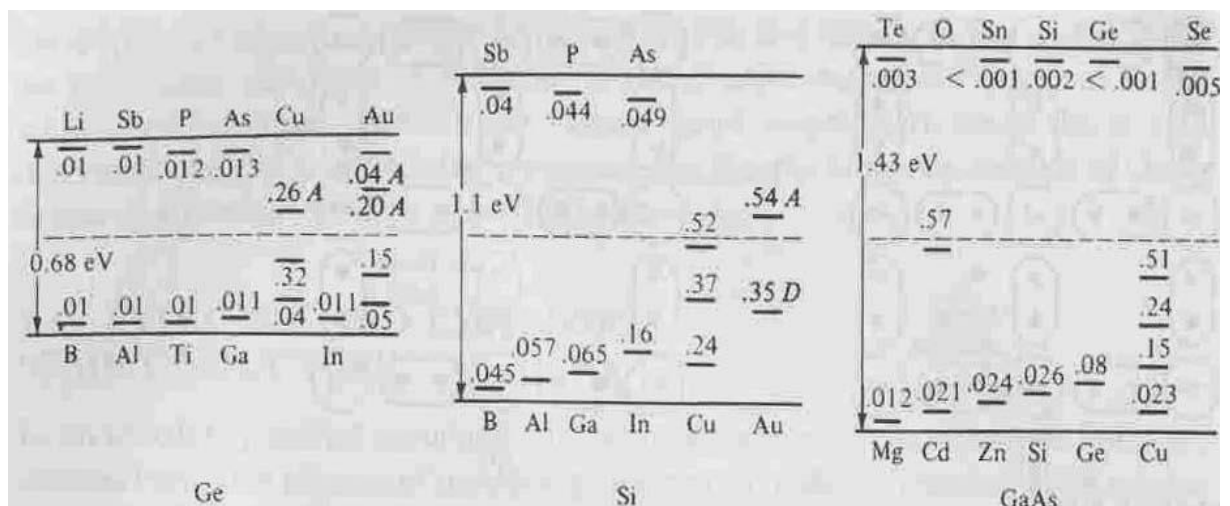


FIGURE 1-15

Ionization energies for various impurities in Ge, Si, and GaAs at 300 K. (After Sze [4].)

- usually most impurity atoms introduce a single energy level, however, interaction between host and impurity atoms may give rise to multiple impurity levels (ex Au, Cu)