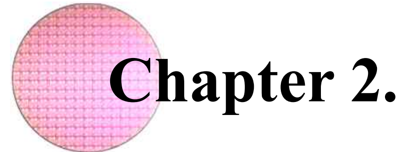

Chapter 2.

Carrier Modeling

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Contents

- The Quantization Concept
- Semiconductor Models
- Carrier Properties
- State and Carrier Distributions
- Equilibrium Carrier Concentrations

✓Carriers: electron, hole

✓ Equilibrium: no external voltages, magnetic fields, stresses, or other perturbing forces acting on the semiconductor. All observables are invariant with time.

- The Quantization Concept

✓ In 1913 Niels Bohr hypothesized that "quantization" of the electron's angular momentum was coupled directly to energy quantization

$$E_{\mathrm{n}} = -\frac{m_0 q^2}{2(4\pi\varepsilon_0 \mathbf{n}\hbar)^2} = -\frac{13.6}{\mathbf{n}^2} \quad \text{eV}, \qquad \text{n=1, 2, 3, } \cdots$$

n is the energy quantum number or orbit identifier

The *electron volt* (eV) is a unit of energy equal to 1.6×10^{-19} joules

The hydrogen atom – idealized representation showing the first three allowed electron orbits and the associated energy quantization

n = 1
–13.6 eV
n = 2
–3.4 eV
n = 3
E_H = –1.51 e

n = 2
8 Electrons
+14
n = 1
2 Electrons
Six allowed levels at same energy
Two allowed levels at same energy
s p
n = 3

Figure 2.2 Schematic representation of an isolated Si atom.

❑ Semiconductor Models

• Bonding Model

✓ Si atoms incorporated in the diamond lattice exhibit a bonding that involves an attraction between each atom and its four nearest neighbors

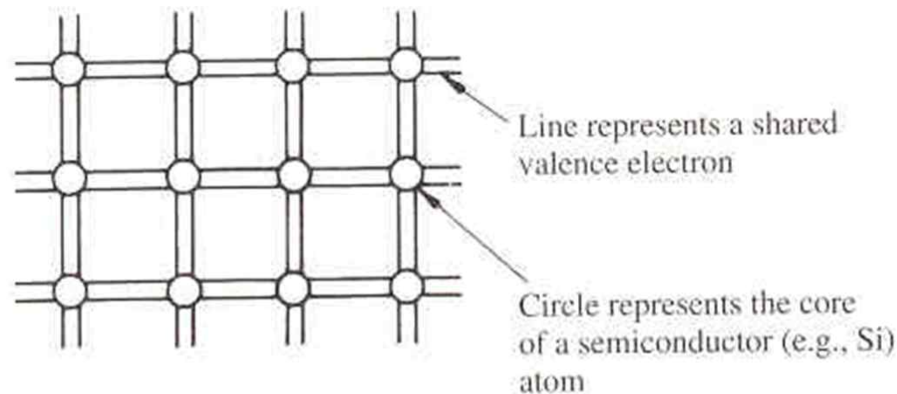

Figure 2.3 The bonding model.

✓ Any given atom not only contributes four shared electrons but must also accept four shared electrons from adjacent atoms

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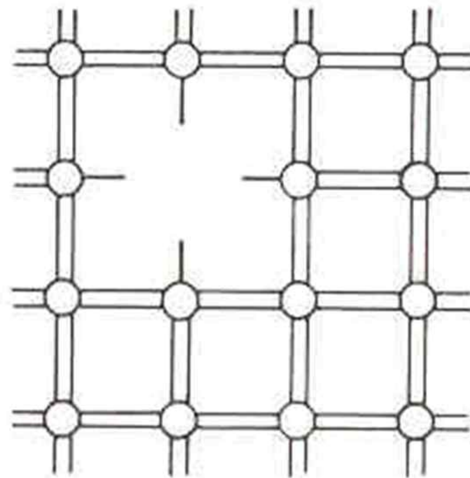
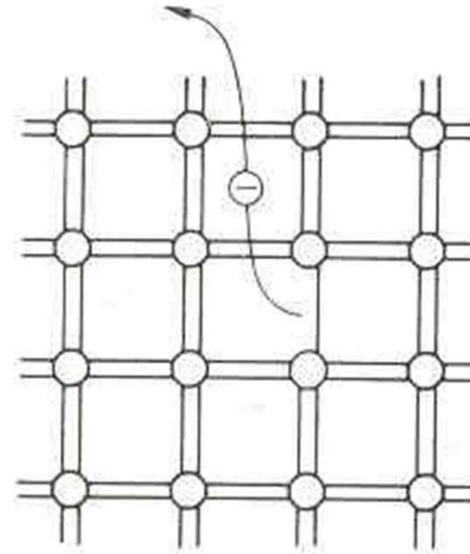




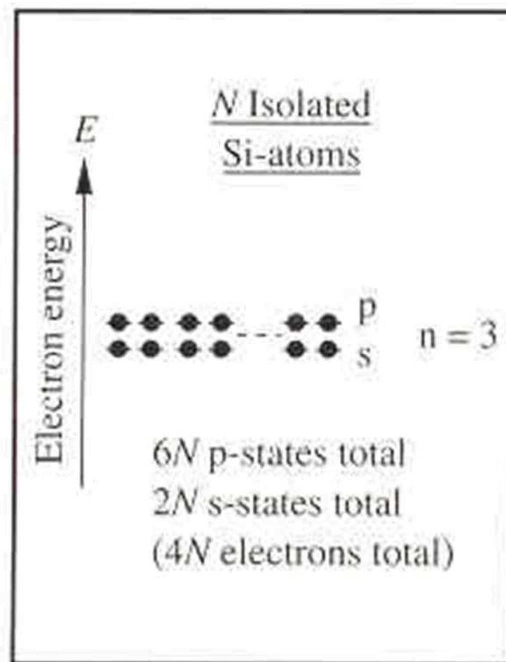
Visualization of a missing atom or point defect

Breaking of an atom-to-atom bond and freeing of an electron

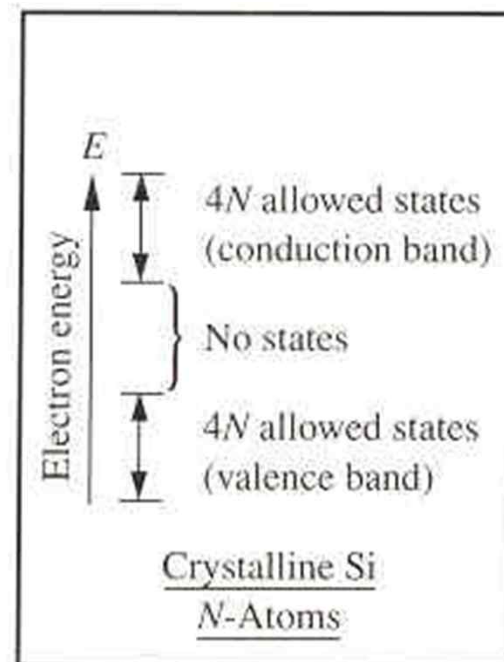
- Energy Band Model
  - ✓ Starting with N-isolated Si atoms, and conceptually bringing the atoms closer and closer together, Pauli exclusion principle makes a progressive spread in the allowed energies

✓ Energy bands: the spread in energies gives rise to closely spaced sets of allowed states → conduction band, valence band, band gap (or forbidden gap)

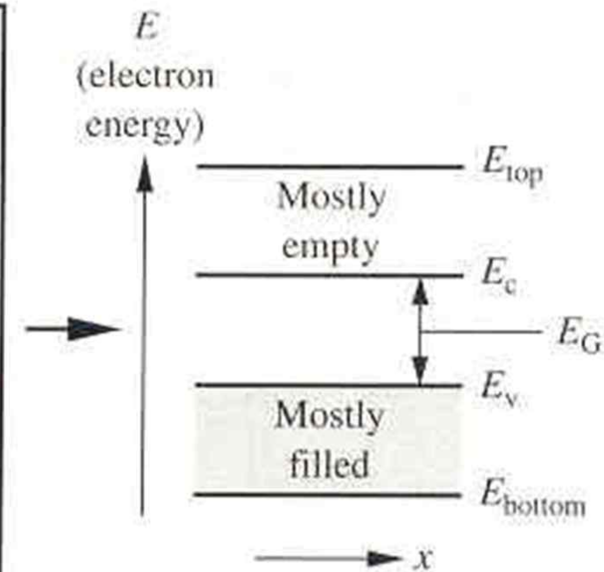
✓ In filling the allowed energy band states, electrons tend to gravitate to the lowest possible energies



Isolated Si atoms

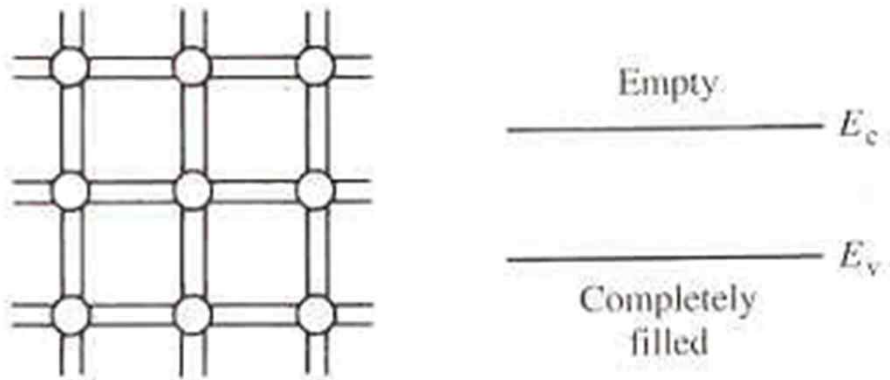


Si lattice spacing

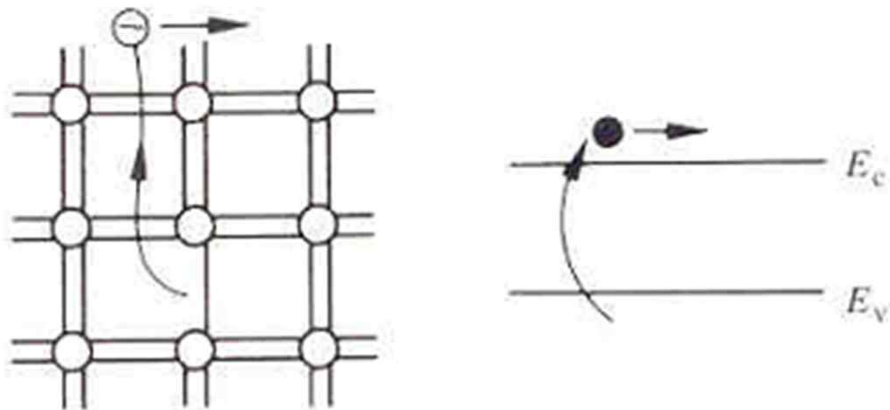


✓ The valence band is almost completely filled with electrons and the conduction band is all but devoid of electrons
✓ The valence band is completely filled and the conduction band completely empty at temperatures approaching T=0 K

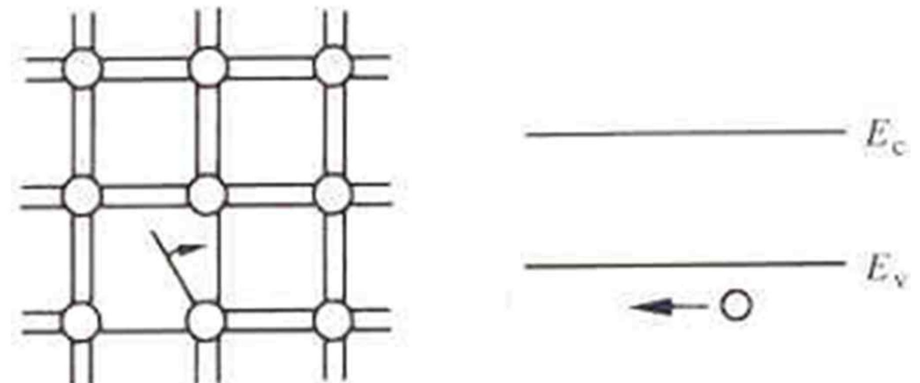
- Carriers
  - ✓ When a Si-Si bond is broken and the associated electron is free to wander, the released electron is a carrier
  - ✓ In terms of the band model, excitation of valence band electrons into the conduction band creates carriers; *electrons in the conduction band are carriers*
  - ✓*Completely filled valence band : no current*
  - ✓The breaking of a Si-Si bond creates a missing bond or void
  - ✓ Missing bond in the bonding scheme, the empty state in the valence band, is the second type of carrier– the hole
  - ✓ Both electrons and holes participate in the operation of most semiconductor devices



(a) No carriers

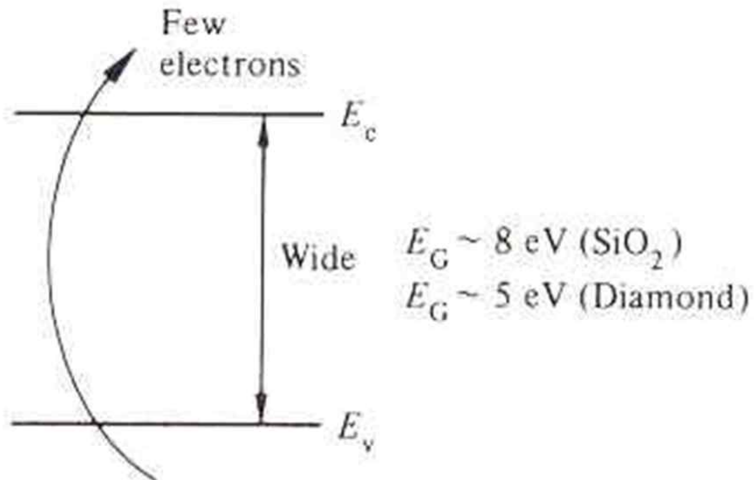


(b) The electron

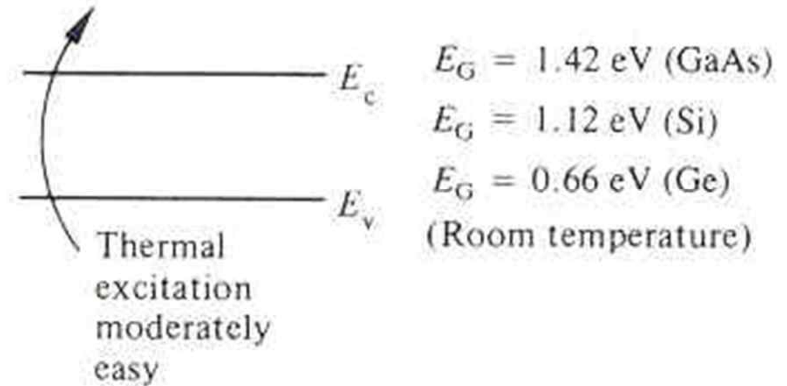


(c) The hole

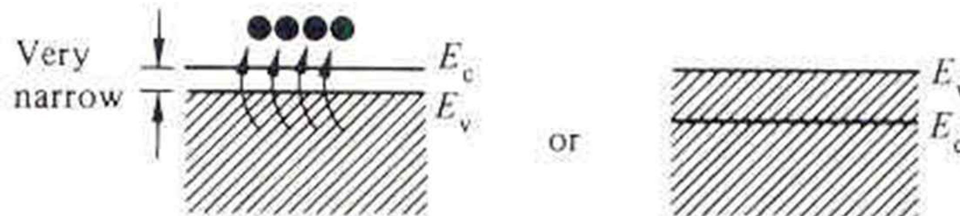
- Band Gap and Material Classification
  - ✓ The major difference between materials lies not in the nature of the energy bands, but rather in the magnitude of the energy gap
  - ✓ Insulators: wide band gap. The thermal energy available at room temperature excites very few electrons from the valence band into the conduction band; thus very few carriers exist inside the material
  - ✓ Metals: very small or no band gap exists at all due to an overlap of the valence and conduction bands. An abundance of carriers → excellent conductors
  - ✓ Semiconductors; intermediate case
  - ✓ At 300K, E_G=1.42 eV in GaAs, E_G=1.12 eV in Si, E_G=0.66 eV in Ge.
  - ✓ Thermal energy, by exciting electrons from the valence band into the conduction band, creates a moderate number of carriers



(a) Insulator



(b) Semiconductor

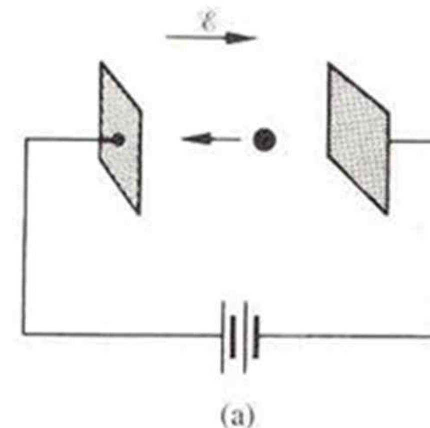


(c) Metal

❑ Carrier Properties

- Charge
  - ✓ Electron (-q), hole (+q), q=1.6×10^{-19} C

- Effective Mass
  - ✓ An electron of rest mass m_0 is moving in a vacuum between two parallel plates under the influence of E,



$$\mathbf{F} = -q\mathbf{E} = m_0 \frac{d\mathbf{v}}{dt}$$

  - ✓ Conduction band electrons moving between the two parallel end faces of a semiconductor crystal under the influence of an applied electric field
  - ✓ Electrons will collide with atoms → a periodic deceleration

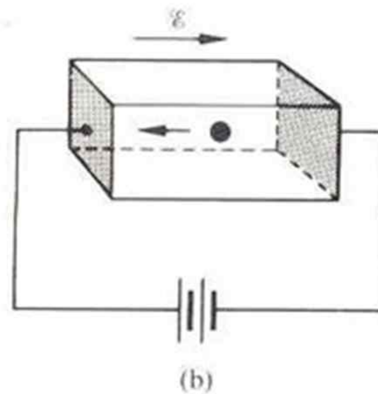
✓ In addition to the applied electric field, electrons in a crystal are also subject to complex crystalline fields

✓The motion of carriers in a crystal can be described by Quantum Mechanics.

✓ If the dimensions of the crystal are large compared to atomic dimensions, the complex quantum mechanical formulation for the carrier motion between collisions simplifies to yield an equation of motion identical to Newton's 2nd equation, except that m_0 is replaced by an effective carrier mass

$$\mathbf{F} = -qE = m_n^* \frac{d\mathbf{v}}{dt}$$

Electron effective mass



✓ For holes with $-q$ → q and $m_n^* \rightarrow m_p^*$

✓ The carrier acceleration can vary with the direction of travel in a crystal → multiple components

✓ Depending on how a macroscopic observable is related to the carrier motion, there are, for example, cyclotron resonance effective masses, conductivity effective masses, density of state effective mass, among others.

Density of State Effective Masses at 300 K

Material	m_n^* / m_0	m_p^* / m_0
Si	1.18	0.81
Ge	0.55	0.36
GaAs	0.066	0.52

- Carrier Numbers in Intrinsic Material
  - ✓ Intrinsic semiconductor = pure (undoped) semiconductor
  - ✓ An intrinsic semiconductor under equilibrium conditions

$$n = p = n_i$$

$$n_i = 1 \times 10^{10}\ cm^{-3} \quad in\ \ Si\ at\ room\ temperature$$

✓ The electron and hole concentrations in an intrinsic semiconductor are equal:

✓ Si atom density: 5×10^{22} cm^{-3}, total bonds: 2×10^{23} cm^{-3} and n_i~ 10^{10} cm^{-3} → 1/10^{13} broken in Si @ 300 K

• Manipulation of Carrier Numbers - Doping

✓ The addition of specific impurity atoms with the purpose of increasing the carrier concentration

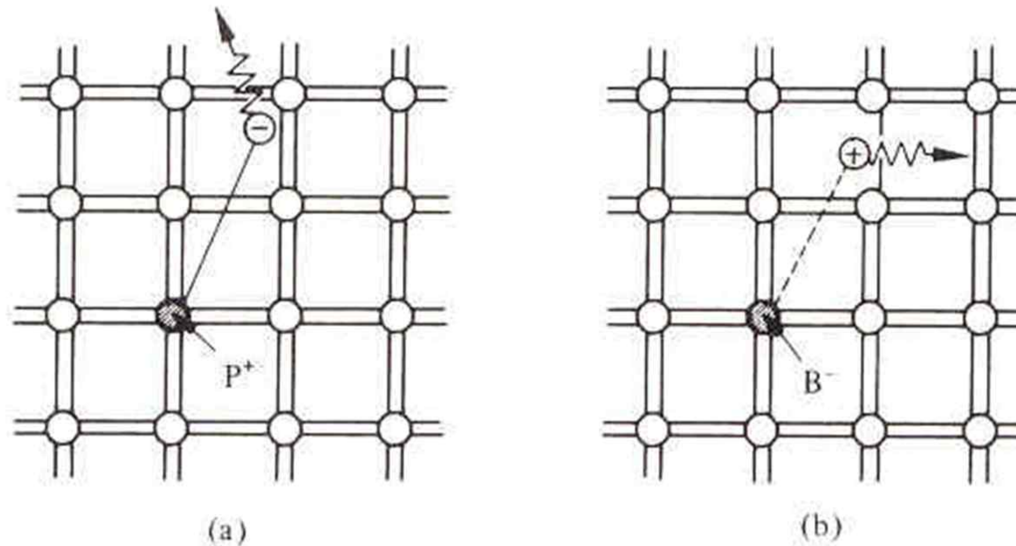
Common Si dopants.

Donors (Electron-increasing dopants)	*Acceptors (Hole-increasing dopants)*
P ← As ← Sb } Column V elements	B ← Ga In Al } Column III elements

✓ Column V element with five valence electrons is substituted for a Si atom , four of the five valence electrons fits snugly into the bonding structure

✓ The fifth donor electron, however, does not fit into the bonding structure and is weakly bound

✓ At 300 K, the donor electron is readily freed to wander hence becomes a carrier (!! no hole generation)
✓ The positively charged donor ion left behind (cannot move)

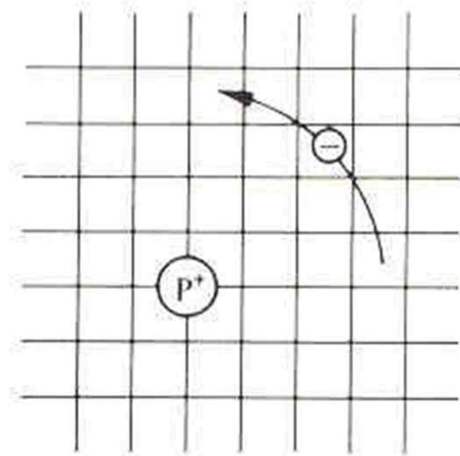


✓ The Column III acceptors have three valence electrons and cannot complete one of the bonds.

✓ The Column III atom readily accepts an electron from a nearby bond, thereby completing its own bonding scheme and in the process creating a hole that can wander

✓ The negatively charged acceptor ion cannot move, and no electrons are released in the hole-creation process

✓ Weakly bound? : a binding energy ~0.1 eV or less



The positively charged donor-core-plus-fifth electron may be likened to a hydrogen atom

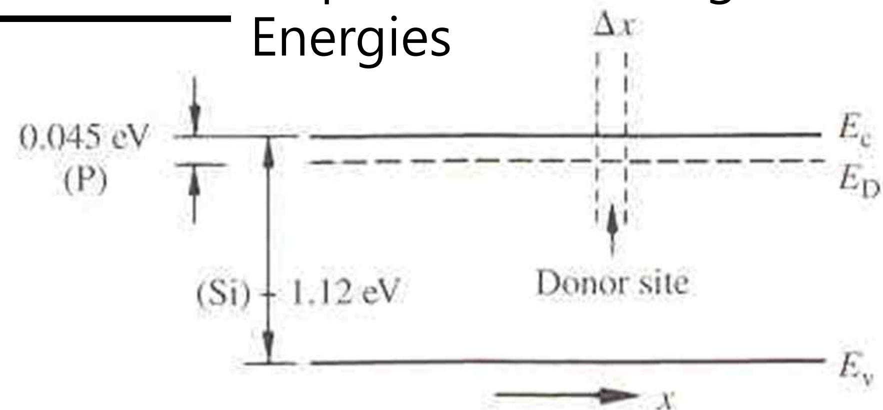
$$\varepsilon_r = K_S = 11.8$$

$$E_B \cong -\frac{m_n^* q^4}{2(4\pi K_S \varepsilon_0 \hbar)^2} = \frac{m_n^*}{m_0}\frac{1}{K_S^2} E_{H|\mathbf{n}=1} \cong -0.1 \text{ eV}$$

Donors	$\lvert E_B \rvert$	Accepters	$\lvert E_B \rvert$
Sb	0.039eV	B	0.045eV
P	0.045eV	Al	0.067eV
As	0.054eV	Ga	0.072eV
		In	0.16eV

Table 2.3

Dopant-Site Binding Energies



✓ The bound electron occupies an allowed electronic levels at an energy $E_D=E_c-|E_B|$

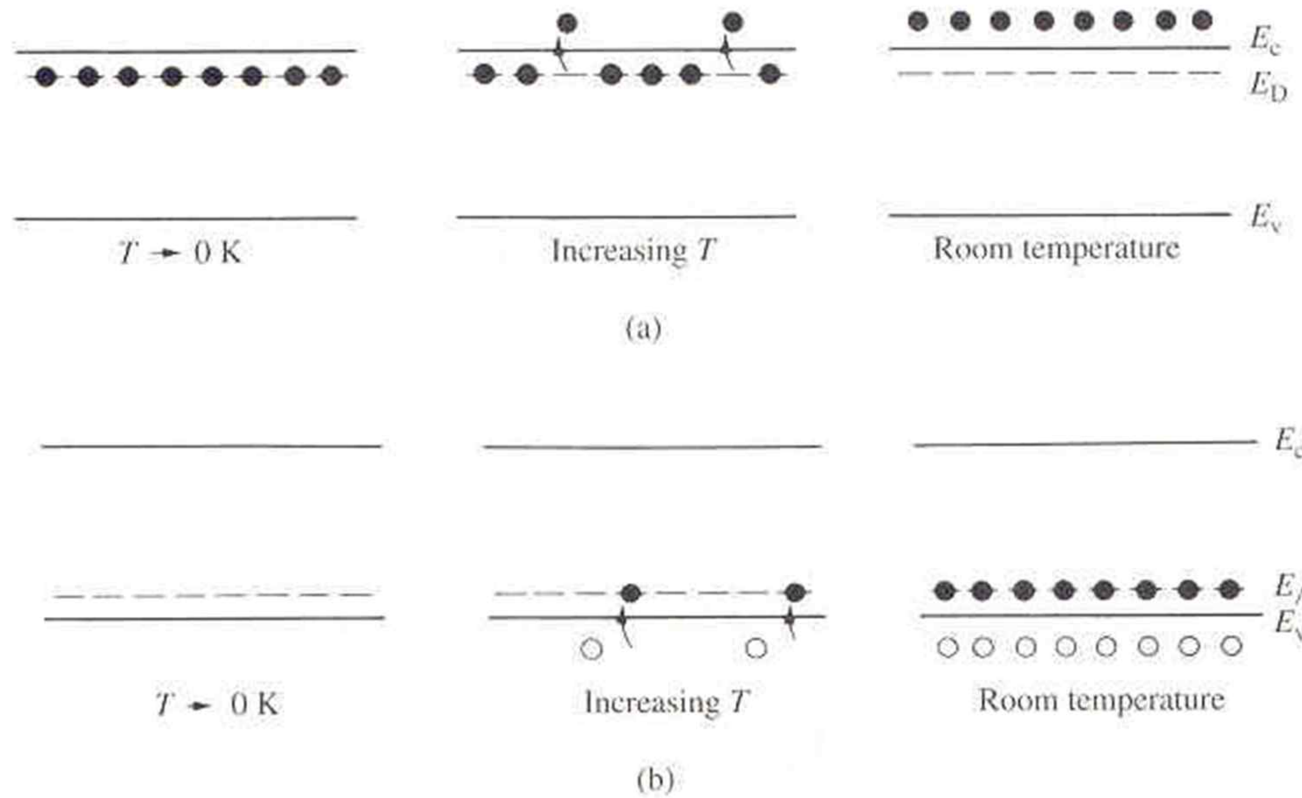
$$E_c - E_D = |E_B| \cong (1/20)E_G(\mathrm{Si})$$

✓ All donor sites filled with bound electrons at T→ 0 K

✓ As the temperature is increased, with more and more of the weakly bound electrons being donated to the conduction band

✓ At 300 K, the ionization is all but total

✓ The situation for acceptors is completely analogous



Visualization of (a) donor and (b) acceptor action using the energy band model

Δx

0.045 eV
(P)

E_C

E_D

Donor site

(Si) 1.12 eV

T = 300 K

E_V

x

- Carrier-Related Terminology
  - ✓ *Dopants*: specific impurity atoms that are added to semiconductors in controlled amounts for the purpose of increasing either the electron or the hole concentration
  - ✓ *Intrinsic semiconductor*: undoped semiconductor
  - ✓ *Extrinsic semiconductor*: doped semiconductor
  - ✓ *Donor*: impurity atom that increases the electron concentration
  - ✓ *Acceptor*: impurity atom that increases the hole concentration
  - ✓ *n-type material*: a donor-doped material
  - ✓ *p-type material*: a acceptor-doped material
  - ✓ *Majority carrier*: the most abundant carrier in a given semiconductor sample; electron in an n-type material and hole in a p-type material
  - ✓ *Minority carrier*: the least abundant carrier in a given semiconductor sample; holes in an n-type material and electrons in a p-type material

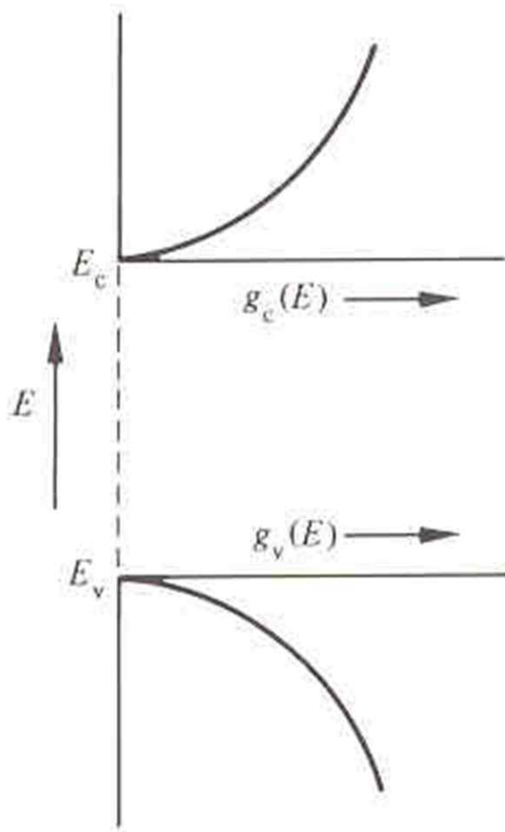
❑ State and Carrier Distributions

- Density of States
  - ✓ How many states are to be found at any given energy in the energy bands?
  - ✓ The state distribution is an essential component in determining carrier distributions and concentrations
  - ✓ The results of an analysis based on quantum mechanical consideration: density of states at an energy *E*

$$g_c(E) = \frac{m_n^* \sqrt{2m_n^*(E - E_c)}}{\pi^2 \hbar^3}, \qquad E \geq E_c$$

$$g_v(E) = \frac{m_p^* \sqrt{2m_p^*(E_v - E)}}{\pi^2 \hbar^3}, \qquad E \leq E_v$$

Difference between $g_c(E)$ and $g_v(E)$ stem from differences in the masses.



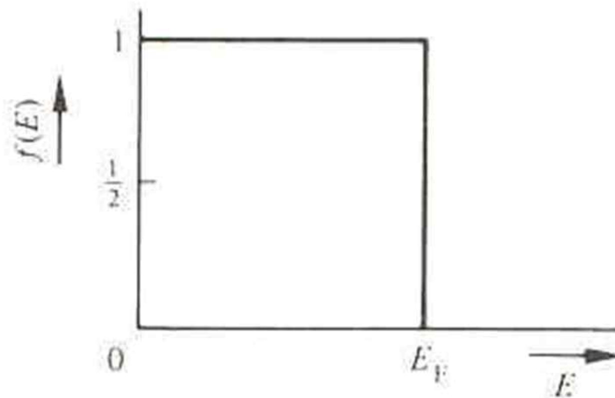
$g_c(E)dE$ represents the number of conduction band states/cm^3 lying in the energy range between *E* and *E*+*dE*

$g_v(E)dE$ represents the number of valence band states/cm^3 lying in the energy range between *E* and *E*+*dE*

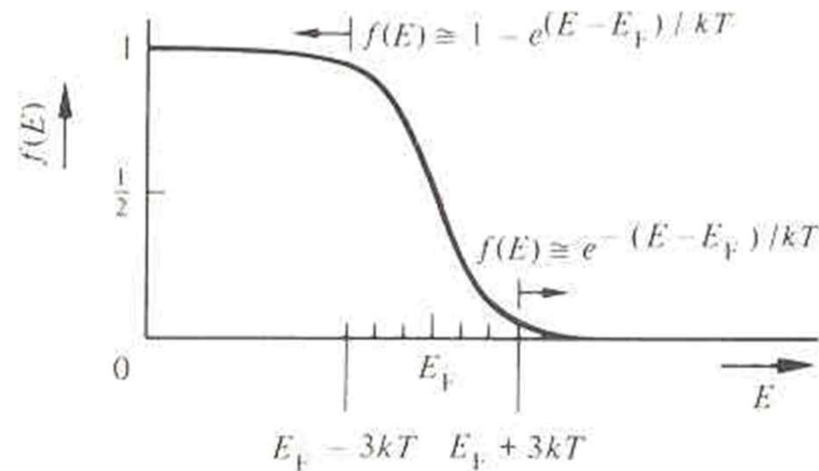
- The Fermi Function
  - ✓ $g(E)$ tells one how many states exist at a given energy *E*
  - ✓ Fermi function *f(E)* specifies the probability that an available state will be occupied by an electron

$$f(E)=\frac{1}{1+e^{(E-E_F)/kT}}$$

E_F=Fermi energy
k=Boltzmann constant (*k*=8.617×10-5 eV/K)
T = temperature



(a) $T \to 0$ K



(b) $T > 0$ K

(i) $f(E_F)=1/2$

(ii) If $E \geq E_F + 3kT, e^{(E-E_F)/kT} >> 1$ and $f(E) \cong e^{-(E-E_F)/kT}$

(iii) If $E \leq E_F - 3kT, e^{(E-E_F)/kT} >> 1$ and $f(E) \cong 1 - e^{(E-E_F)/kT}$: $1 - f(E)$ empty

(iv) At T=300 K, kT=0.0259 eV and $3kT$=0.0777 eV << E_G

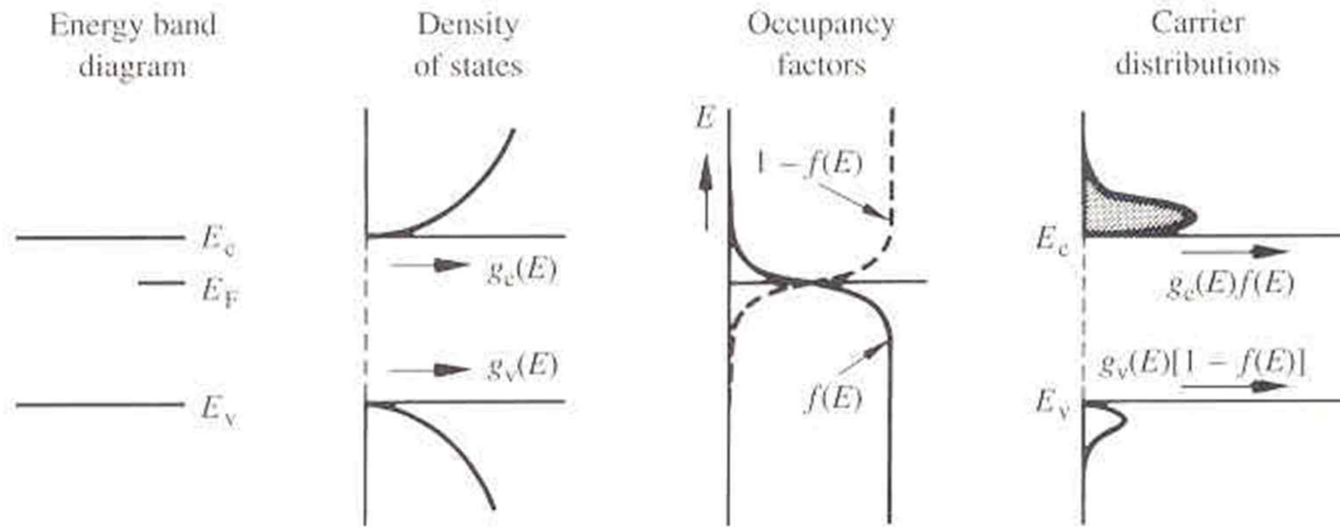
- Equilibrium Distribution of Carriers

$$g_c(E)f(E) \;\; \& \;\; g_v(E)[1-f(E)]$$

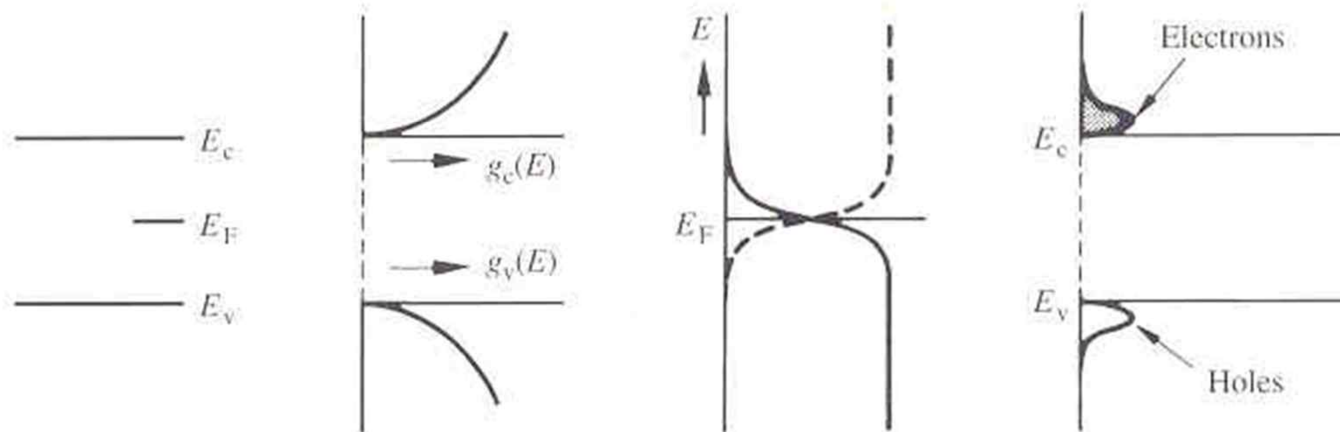
✓ All carrier distributions are zero at the band edges, reach a peak value very close to E_c or E_v

✓When E_F is positioned in the upper half of the band gap (or higher), the electron distribution greatly outweighs the hole distribution

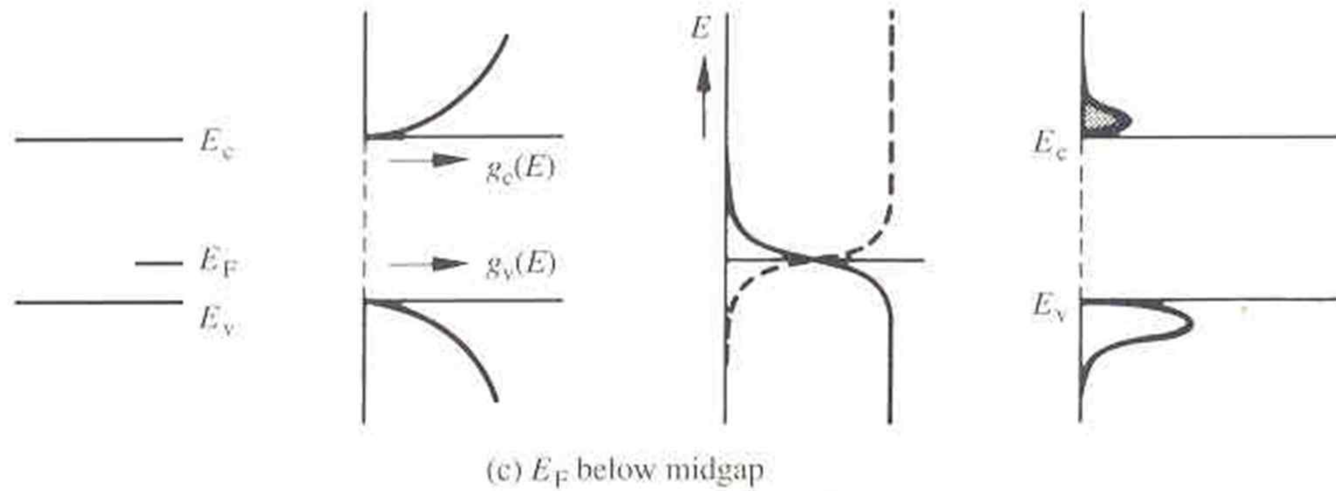
✓ Equal number of carriers when E_F is at the middle



(a) E_F above midgap

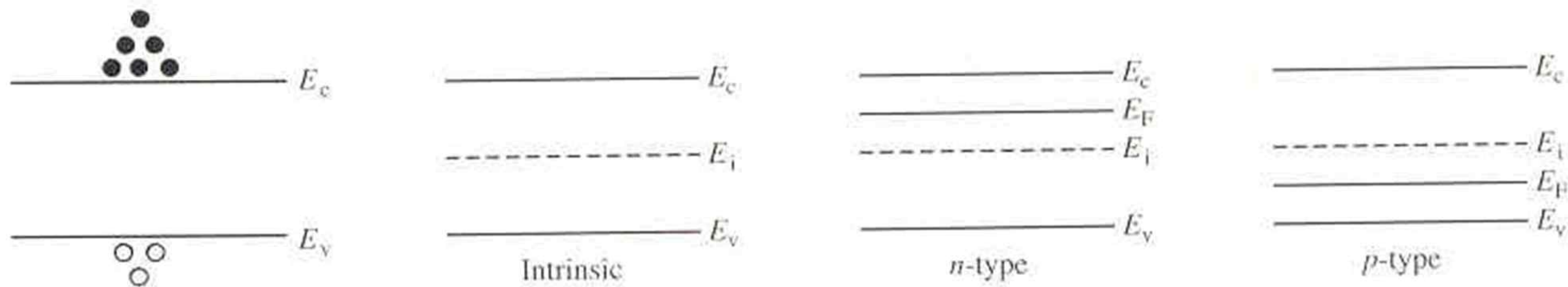


(b) E_F near midgap



(c) E_F below midgap

✓ Abbreviated fashion; The greatest number of circles or dots are drawn close to E_c and E_v, reflecting the peak in the carrier concentrations near the band edges



❑ Equilibrium Carrier Concentrations

- Formulas for *n* and *p*
  - ✓ $g_c(E)f(E)dE$: the number of conduction band electrons/cm^3 lying in the *E* to *E*+*dE* range

$$n = \int_{E_c}^{E_{top}} g_c(E) f(E) dE$$

$$p = \int_{E_{botton}}^{E_v} g_v(E)\left[1 - f(E)\right] dE$$

  - ✓ For n-type material

$$n = \frac{m_n^* \sqrt{2m_n^*}}{\pi^2 \hbar^3} \int_{E_c}^{E_{top}} \frac{\sqrt{E - E_c}\; dE}{1 + e^{(E - E_F)/kT}}$$

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✓ Defining

$$N_C = 2\left[\frac{m_n^* kT}{2\pi\hbar^2}\right]^{3/2}, \quad \text{the "effective" density of conduction band states}$$

$$N_V = 2\left[\frac{m_p^* kT}{2\pi\hbar^2}\right]^{3/2}, \quad \text{the "effective" density of valence band states}$$

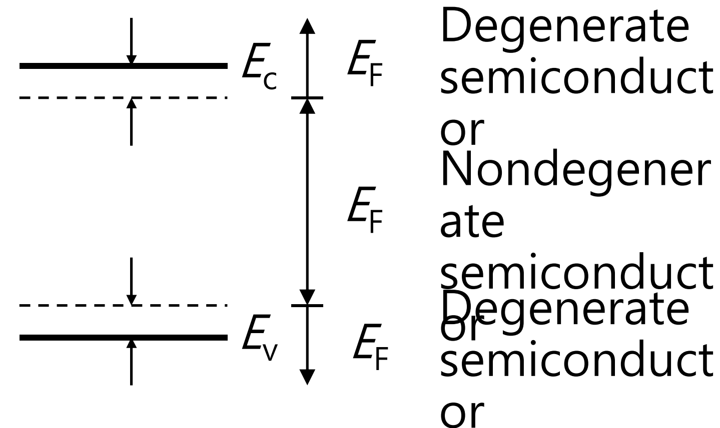
✓ At 300 K

$$N_{C,V} = (2.510 \times 10^{19}\ \text{cm}^{-3})(m_{n,p}^* / m_0^*)$$

✓ If $E_v + 3kT \le E_F \le E_c - 3kT$

$$n = N_C e^{(E_F - E_c)/kT}$$

$$p = N_V e^{(E_v - E_F)/kT}$$



*Alternative Expressions for n and p

✓ For intrinsic semiconductor, $E_i = E_F$

$$n_\mathrm{i} = N_\mathrm{C} e^{(E_\mathrm{i} - E_\mathrm{c})/kT} \quad \rightarrow N_\mathrm{C} = n_i e^{(E_\mathrm{c} - E_\mathrm{i})/kT}$$

$$n_\mathrm{i} = N_\mathrm{V} e^{(E_\mathrm{v} - E_\mathrm{i})/kT} \quad \rightarrow N_\mathrm{V} = n_i e^{(E_\mathrm{i} - E_\mathrm{v})/kT}$$

$$n = n_\mathrm{i} e^{(E_\mathrm{F} - E_\mathrm{i})/kT}$$

$$p = n_\mathrm{i} e^{(E_\mathrm{i} - E_\mathrm{F})/kT}$$

- n_i and the *np* Product

$$n_\mathrm{i}^2 = N_\mathrm{C} N_\mathrm{V} e^{-(E_\mathrm{c} - E_\mathrm{v})/kT} = N_\mathrm{C} N_\mathrm{V} e^{-E_\mathrm{G}/kT}$$

$$n_\mathrm{i} = \sqrt{N_\mathrm{C} N_\mathrm{V}}\, e^{-E_\mathrm{G}/2kT}$$

$$np = n_\mathrm{i}^2$$

Intrinsic carrier concentrations in Ge, Si, and GaAs as a function of temperature

- Charge Neutrality Relationship
  - ✓ For the uniformly doped material to be everywhere charge-neutral clearly requires

$$\frac{\text{charge}}{\text{cm}^3} = qp - qn + qN_\text{D}^+ - qN_\text{A}^- = 0$$

$$p - n + N_\text{D}^+ - N_\text{A}^- = 0$$

N_D^+ = number of ionized donors/cm^3

N_A^- = number of ionized acceptors/cm^3

N_D = total number of donors/cm^3

N_A = total number of acceptors/cm^3

$$\boxed{p - n + N_\text{D} - N_\text{A} = 0}$$

assumes total ionization

- Carrier Concentration Calculations
  - ✓ Assumptions: nondegeneracy and total ionization of dopant atoms

Two equations and two unknowns

$$p = \frac{n_i^2}{n}$$

$$\frac{n_i^2}{n} - n + N_D - N_A = 0$$

$$n^2 - n(N_D - N_A) - n_i^2 = 0$$

$$n = \frac{N_D - N_A}{2} + \left[\left(\frac{N_D - N_A}{2}\right)^2 + n_i^2\right]^{1/2}$$

$$p = \frac{N_A - N_D}{2} + \left[\left(\frac{N_A - N_D}{2}\right)^2 + n_i^2\right]^{1/2}$$

✓ Intrinsic semiconductor (N_A=0, N_D=0) → $n=p=n_i$

✓ Doped semiconductor where either $N_D-N_A \approx N_D >> n_i$ or $N_D-N_A \approx N_A >> n_i$ (usual)

$$\boxed{\begin{array}{l} n \approx N_D \\ p \approx n_i^2 / N_D \end{array}} \qquad N_D >> N_A, \quad N_D >> n_i$$

(nondegenerate, total ionization)

$$\boxed{\begin{array}{l} p \approx N_A \\ n \approx n_i^2 / N_A \end{array}} \qquad N_A >> N_D, \quad N_A >> n_i$$

(nondegenerate, total ionization)

- Determination of E_F
  - ✓ one-to-one correspondence between E_F and the n & p
  - ✓Exact positioning of E_i

$$n = p$$

$$N_C e^{(E_i - E_c)/kT} = N_V e^{(E_v - E_i)/kT}$$

$$E_i = \frac{E_c + E_v}{2} + \frac{kT}{2} \ln\left(\frac{N_V}{N_C}\right)$$

$$\frac{N_V}{N_C} = \left(\frac{m_p^*}{m_n^*}\right)^{3/2}$$

$$\boxed{E_i = \frac{E_c + E_v}{2} + \frac{3}{4} kT \ln\left(\frac{m_p^*}{m_n^*}\right)}$$

$$(3/4)kT \ln(m_p^* / m_p^*) = -0.0073 \text{ eV}$$

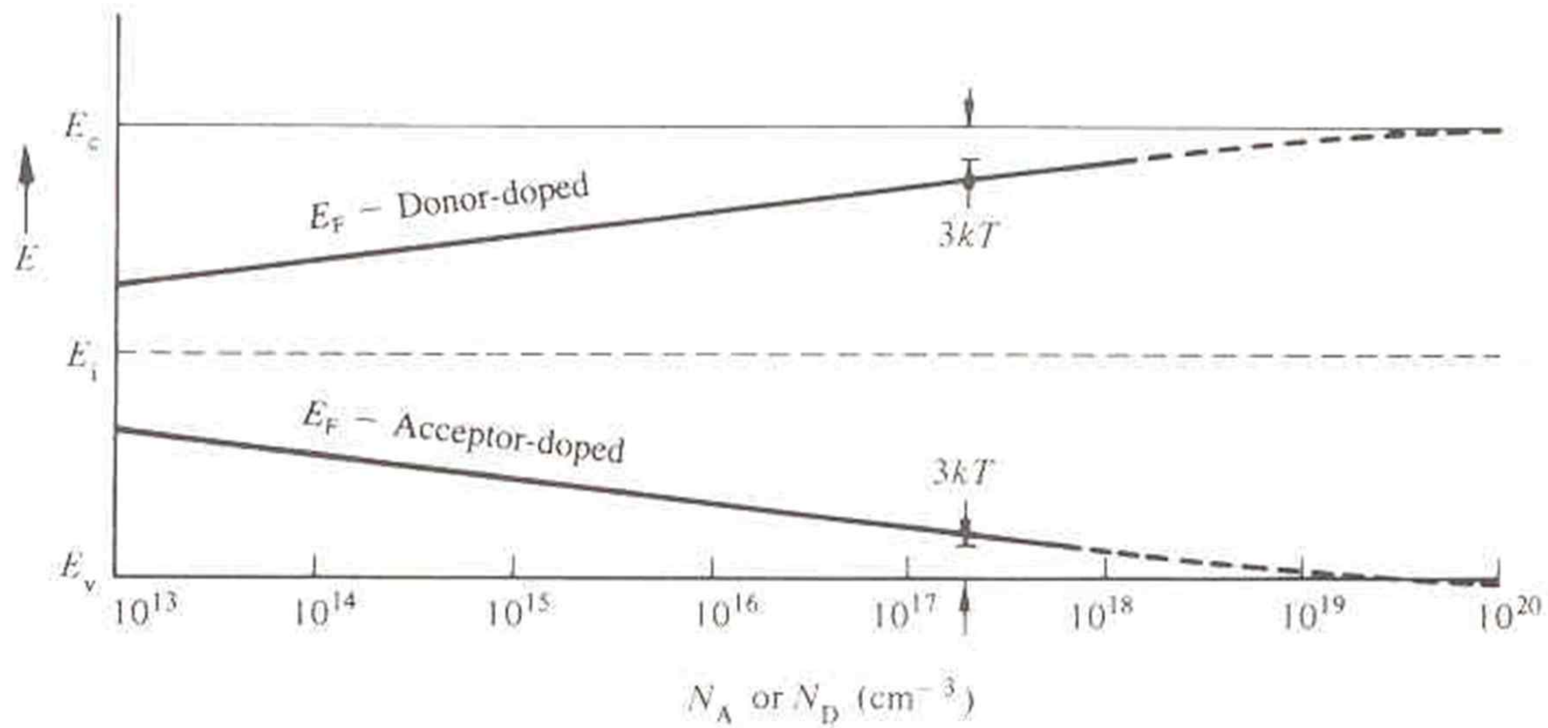
✓ Doped semiconductors

$$n = n_i e^{(E_F - E_i)/kT}$$

$$E_\mathrm{F} - E_\mathrm{i} = kT \ln(n/n_\mathrm{i}) = -kT \ln(p/n_\mathrm{i})$$

$$n \cong N_D \ \text{ for n-type semiconductors}$$
$$p \cong N_A \ \text{ for p-type semiconductors}$$

$$\boxed{\begin{aligned} E_\mathrm{F} - E_\mathrm{i} &= kT \ln(N_\mathrm{D}/n_\mathrm{i}) \\ E_\mathrm{i} - E_\mathrm{F} &= kT \ln(N_\mathrm{A}/n_\mathrm{i}) \end{aligned}}$$



The maximum nondegenerated doping concentrations

$$N_D \cong 1.6 \times 10^{18} / cm^3$$

$$N_A \cong 9.1 \times 10^{17} / cm^3$$

Summary

Ch2. 9/28/10

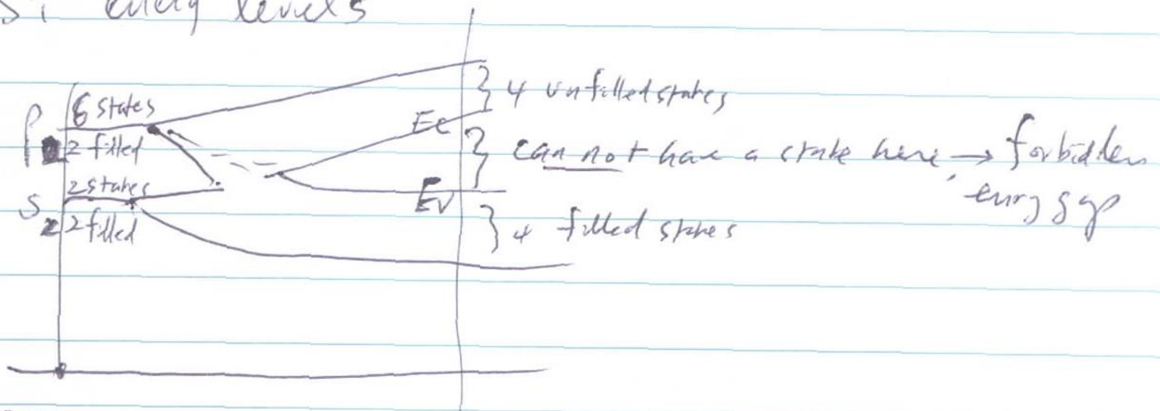
Quantization: energy levels are quantized!
Bohr's Model

$$E_H = -\frac{m_0 q^4}{2(4\pi\epsilon_0 \hbar n)^2} = -\frac{13.6\,eV}{n^2}$$

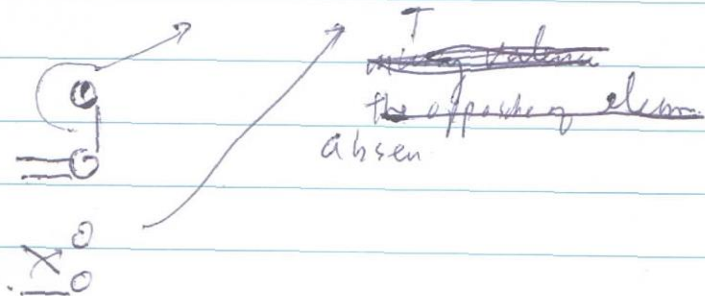
Semiconductor - Bonding Model
4 valence electrons
shared by 4 neighbors.

Missing link = electron + hole

~~Energy~~
~~Energy~~
Si energy levels



carriers : electrons + holes



The Bandgap — the size of it determines Material type

~~Conductor~~ Insulator	Semiconductor	Metal
too much	~ 1eV	too little

2.3 carrier properties

Charge $q = 1.6\times10^{-19}$ coul electron q, hole $-q$

Effective Mass

How they behave as in classical mechanical particle, while they are quantum mechanical carriers moving through crystal lattice

$$F = -q\mathcal{E} = m^* \frac{dv}{dt}$$

# of carriers

n, p

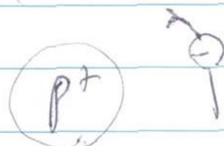
Intrinsic conc. (equilibrium) $n_i = n = p$

only by thermal excitation, electrons & holes are created.

Doping ; control of # of carriers

Group III & V elements for Si,

binding energy — like taking an electron out of H atom (of donor site ~~bonding~~)



$$E_B = -\frac{m_n^* q^4}{2(4\pi K_s \epsilon_0 \hbar)^2} = \frac{m_n^*}{m_0}\cdot\frac{1}{K_s^2} E_{H(\text{ion})}$$

$= -0.1eV$

$\approx \frac{1}{20} E_G(Si)$

Table 2-3 for actual values

E_c ______________

- - - - - - - ← to denote local presense of donor state

E_v ______________

at RT, all donors are ionized. (~100%)

<u>Terminologies</u>

P40. intrinsic semicon — : undoped (extremely pure)

extrin " — : intentionally doped

→ by excitation, & by defects present (ST)

Undoped → does not always mean neutral,

because defects can also act as dopants and show either n or p types

{ Majority carrier
{ minority carrier

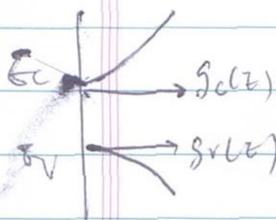
$n \cdot p = n_i^2$ (thermal eq)

(will learn later)

Density of states (also results of Q-M analysis)

in terms of energy

$g_c(E)$ or $g_v(E)$ $\propto \sqrt{E}$ ($\sqrt{E-E_c}$ or $\sqrt{E_v-E}$)



$$g_c(E) = \frac{m_n^* \sqrt{2 m_n^*}}{\pi^2 \hbar^3} \cdot \sqrt{E-E_c} \quad (E \geq E_c)$$

$$g_v(E) = \frac{m_p^* \sqrt{2 m_p^*}}{\pi^2 \hbar^3} \sqrt{E_v-E} \quad (E \leq E_v)$$

Fermi Function:

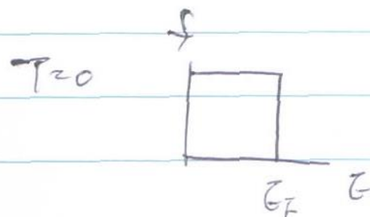
$f(E)$: probability tha a state is filled with an electron under thermal Eq. (T.E.)

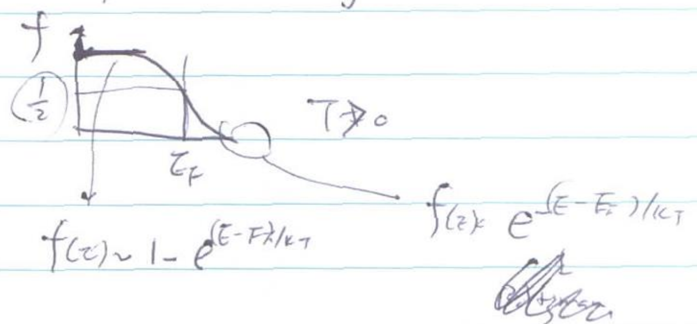
$$f(E) = \frac{1}{1+e^{(E-E_F)/kT}}$$ → a probability distribution fn.

K: Boltzman Const.

T:

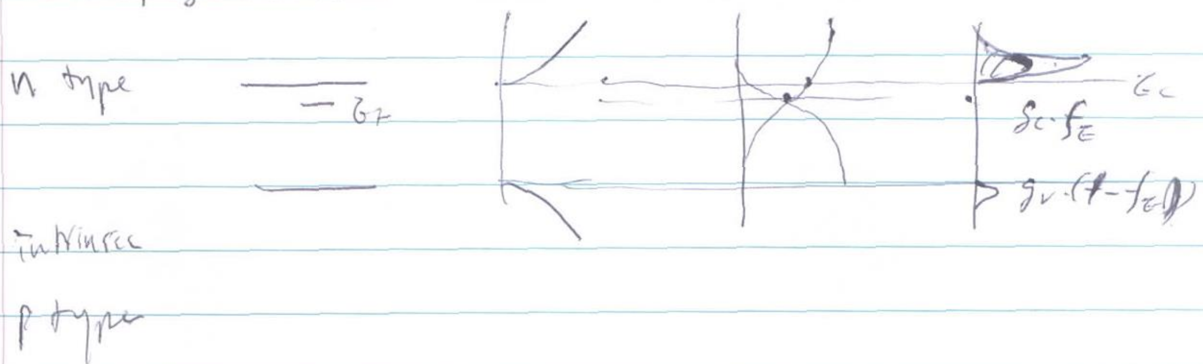
E_F = Fermi Energy level.





Eq. Distribution of Carriers

Figure 2.16



n type

intrinsic

p type

Eqn. Carrier concentrations

$$n = \int_{E_C}^{\infty} g_C(E) f(E)\, dE$$

$$= \frac{m_n^* \sqrt{2m_n^*}}{\pi^2 \hbar^3} \int_{E_C}^{\infty} \frac{\sqrt{E-E_C}}{1+e^{(E-E_F)/kT}}\, dE = N_C \cdot \frac{2}{\sqrt{\pi}} F_{1/2}(\eta_c)$$

$\eta_c = \frac{E_F - E_C}{kT}$

$$= N_C \cdot e^{(E_F-E_C)/kT}$$

N_C: effective density of C-band states

$E_F \leq E_C - 3kT$ only this approximation

$$N_C = 2\left[\frac{m_n^* kT}{2\pi \hbar^2}\right]^{\frac{3}{2}}$$

$E_F - E_C \leq$ ~~3kT~~ 0 always negative (So Big ~~number~~ N_V ~~going~~ getting smaller)

In fact $E_V + 3kT \leq E_F \leq E_C - 3kT$

$N_V \cong 2\times10^{19} \left(\frac{m_n^*}{m_0}\right)^{\frac{3}{2}}$ [cm^{-3}]

3kT E_C

← non-degenerate case

3kT E_V

$$= n_i\, e^{(E_F-E_i)/kT}$$

$(E_F - E_i) \gg kT$

(So small n_i ~~going~~ getting larger)

Likewise

$$p = N_V \cdot e^{(E_V - E_F)/kT}$$

$$= n_i \, e^{(E_i - E_F)/kT}$$

Mass Action Law

↳ $n \cdot p = n_i^2$ (from 2nd expression) ($n = n_i \, e^{(E_F - E_i)/kT}$, $p = n_i \, e^{(E_i - E_F)}$ multiply)

$n_i = \sqrt{N_C N_V} \, e^{-E_G/2kT}$ (from 1st expression)

2.5.4 Charge Neutrality

net charge $= q(p - n + N_D^+ - N_A^-) = 0$

$N_D^+ = N_D$, $N_A^- = N_A$
(assume 100% ionization of dopant atoms)

Carrier conc. calculations

$n_i = 10^{10}$ at 300 K

From $p = \frac{n_i^2}{n}$ &
$p - n + N_D - N_A = 0$ } $\rightarrow n^2 - n(N_D - N_A) - n_i^2 = 0$

2차 방정식의 해 $n = \ldots$

cases
1. Intrinsic
   $n = p = n_i$
2. Doped
   n type : $N_D - N_A \simeq N_D \gg n_i \rightarrow n = N_D$, $p = \frac{n_i^2}{N_D}$
   p type : $N_A - N_D \simeq N_A \gg n_i \rightarrow p = N_A$, $n = \frac{n_i^2}{N_A}$
3. Doped But High Temp.
   (High enough $n_i \gg N_A$ or N_D)
   $n \sim p \sim n_i$
4. $N_A \sim N_D$ Compensated semicon.
   can't ignore either one.

E_F Determination

1) E_i Is $E_i = \frac{E_c + E_v}{2}$? (Roughly Yes.) But,

$n = p$. & $N_c e^{(E_i - E_c)/kT} = N_v e^{(E_v - E_i)/kT}$

$\rightarrow E_i = \frac{E_c + E_v}{2} + \frac{kT}{2} \ln\left(\frac{N_v}{N_c}\right)$

$\left(\frac{N_v}{N_c}\right)$ " $\left(\frac{m_p^*}{m_n^*}\right)^{\frac{3}{2}}$

at RT, -0.0073 eV.

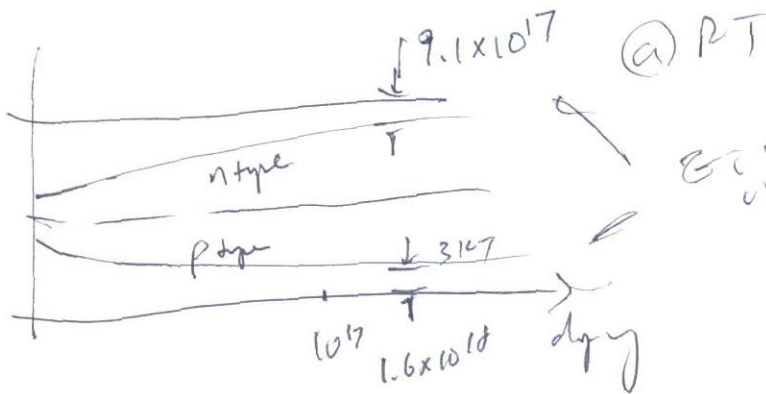
E_F 16

② Doped semi. (non-degenerate, 100% ionization of dopants)

$$n = n_i e^{(E_F - E_i)/kT} \qquad p = n_i e^{(E_i - E_F)/kT}$$

$$\rightarrow E_F - E_i = kT \ln\left(\frac{N_D}{n_i}\right)$$

$$E_i - E_F = +kT \ln\left(\frac{N_A}{n_i}\right)$$



n, p 의 Temp. dependency