EE 3106
Lecture 3

Semiconductor Materials in Equilibrium (I)

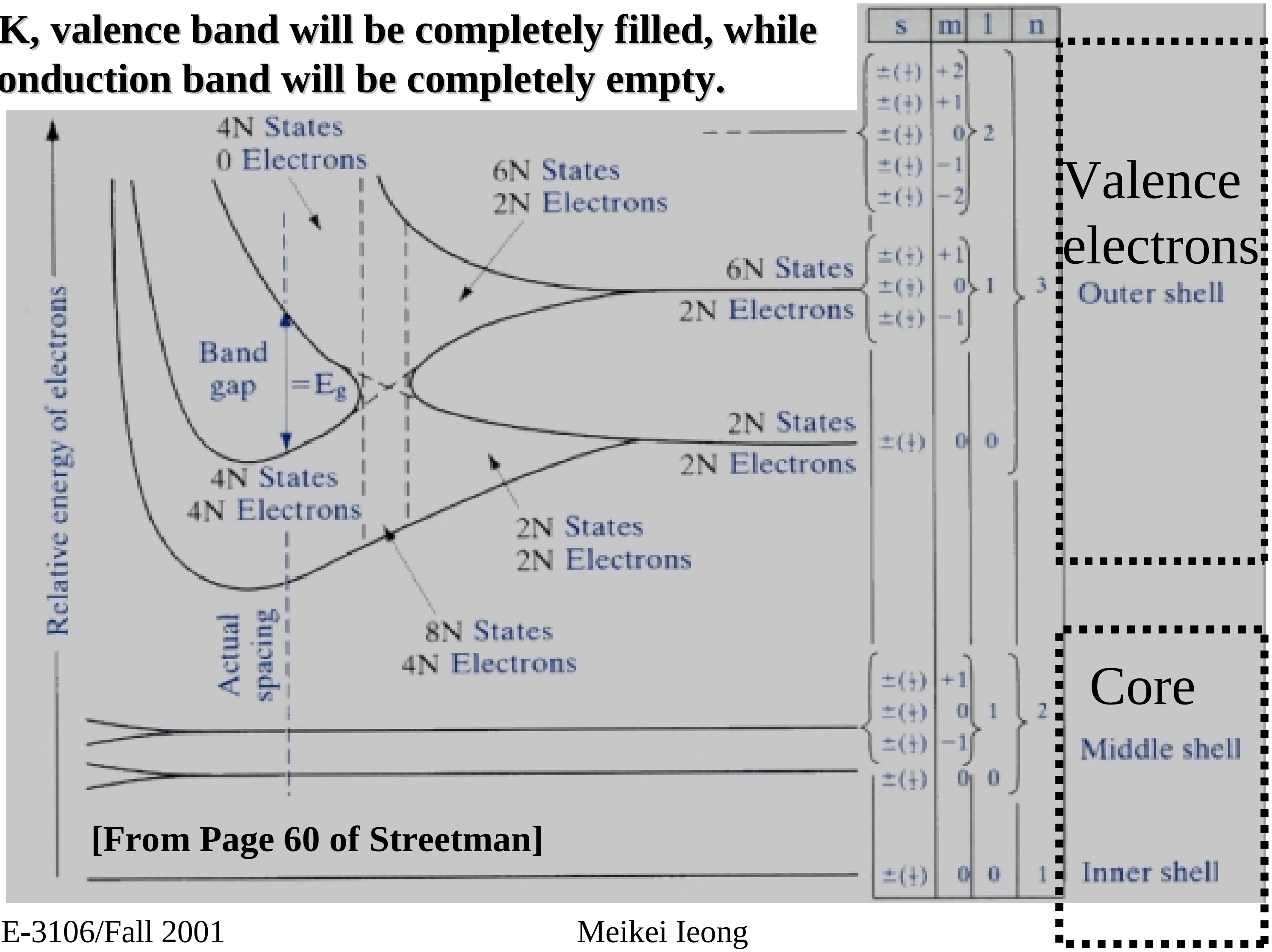
This lecture note can be downloaded from
http://www.ieong.net/ee3106/

The Road Ahead

- Density of States.
- The Fermi Function and Fermi Level.
- Carrier Concentration (Intrinsic and Doped).
- *pn* product, charge neutrality.
- Determination of Fermi-energy, E_F.

Energy Levels in Silicon

There are 4N states in each band.
At 0 K, valence band will be completely filled, while the conduction band will be completely empty.

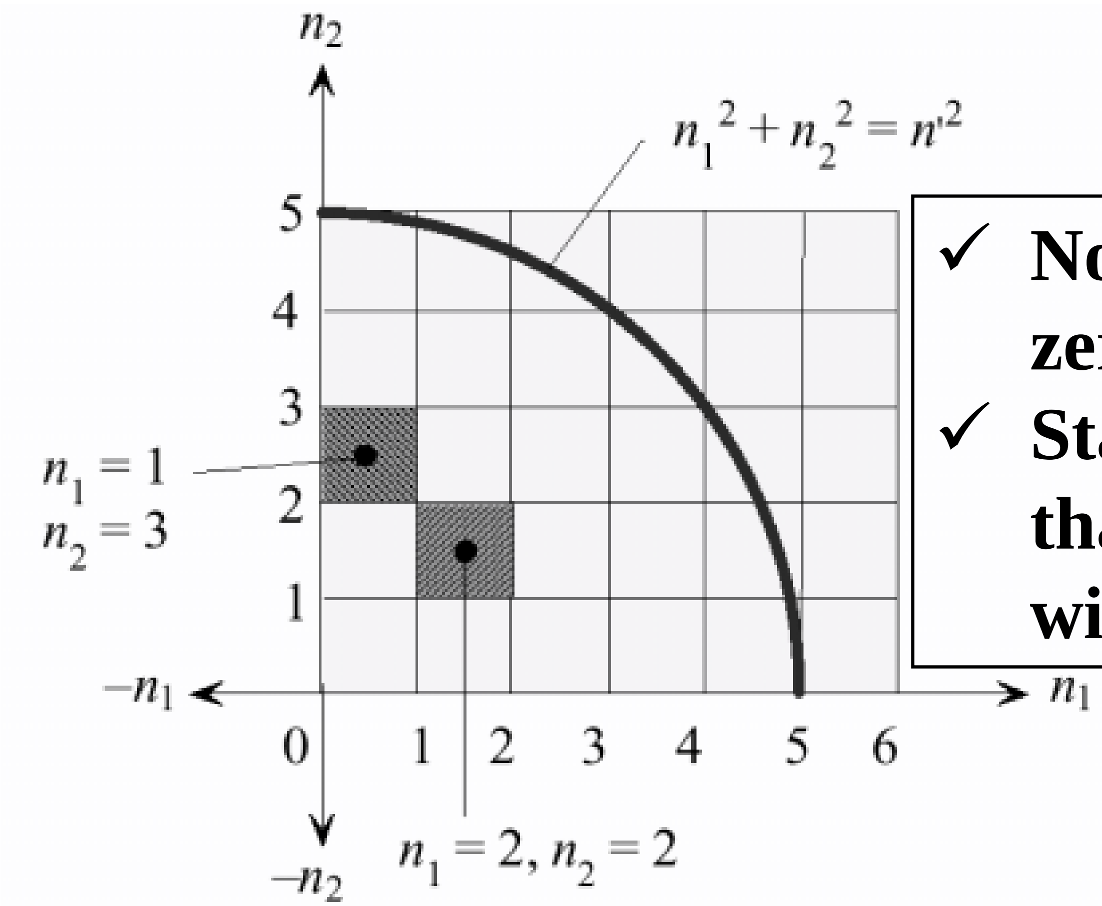


[From Page 60 of Streetman]

Density-of-States

- We are interested in how the allowed energy states are distributed in energy.
- How many allowable states were to be found at any given energy in the conduction and valence bands?
- Essential in determining carrier distributions and concentrations.

Energy States in 2D Square

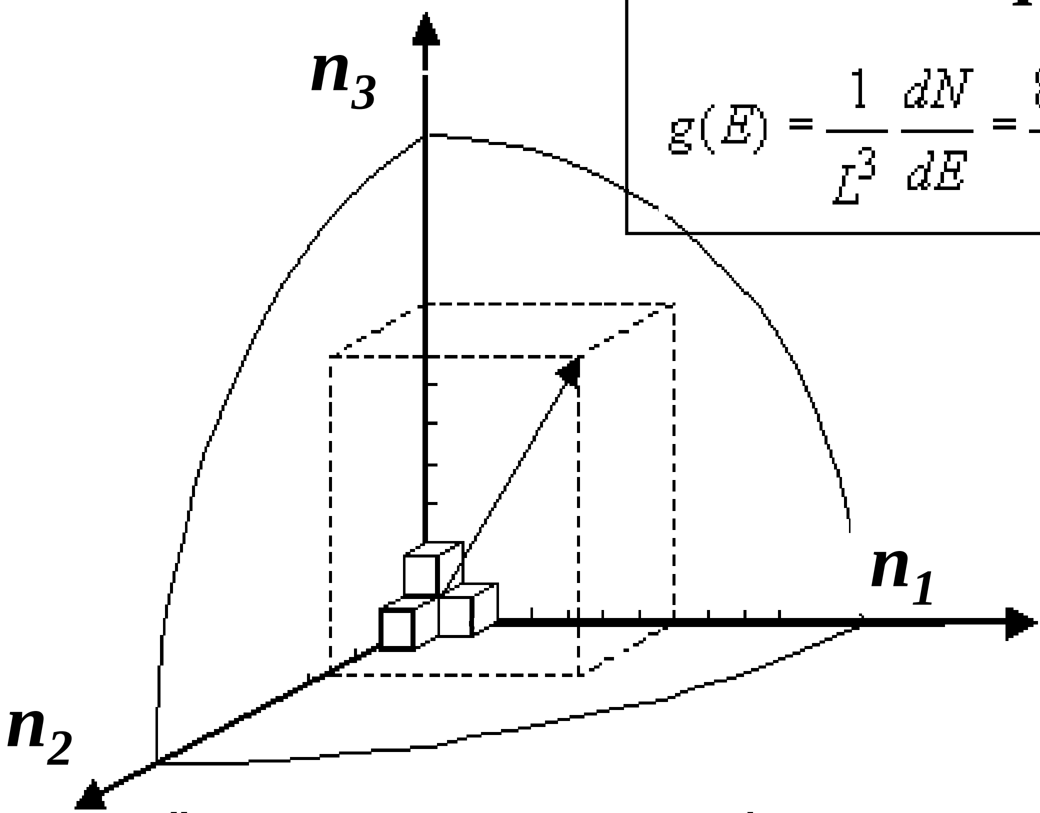


- ✓ **No allowable state at zero energy.**
- ✓ **States with E less than E' will be those with $n_1^2 + n_2^2 < n'^2$**

Energy States in 3D

For Free electrons in a 3D infinite quantum well:

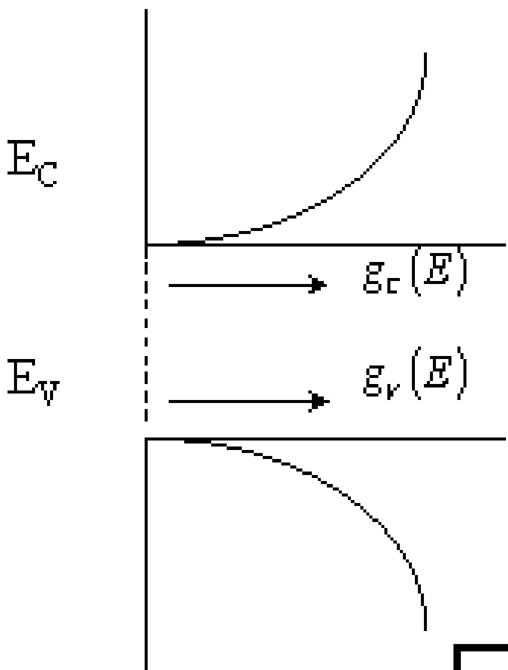
$$g(E) = \frac{1}{L^3}\frac{dN}{dE} = \frac{8\pi\sqrt{2}}{h^3} m^{*3/2}\sqrt{E}, \text{for } E \geq 0$$



Density-of-States in Semiconductors

Density of states at an energy E in the conduction and valence bands

$$\begin{cases} g_c(E) = \dfrac{m_n^* \sqrt{2m_n^*(E - E_C)}}{\pi^2 \hbar^3} & E \geq E_C \\[2ex] g_v(E) = \dfrac{m_p^* \sqrt{2m_p^*(E_V - E)}}{\pi^2 \hbar^3} & E \leq E_V \end{cases}$$



$g_C(E_C) = 0$ $\quad g_C(E)$ — Increases as the square root of the energy when proceeding upward in the conduction band

$g_V(E_V) = 0$ $\quad g_V(E)$ — Increases as the square root of the energy when proceeding downward in the conduction band

Unit: # of states per unit volume per unit energy

Number of Band States

Considering closely spaced energies E and E+dE in the respective bands

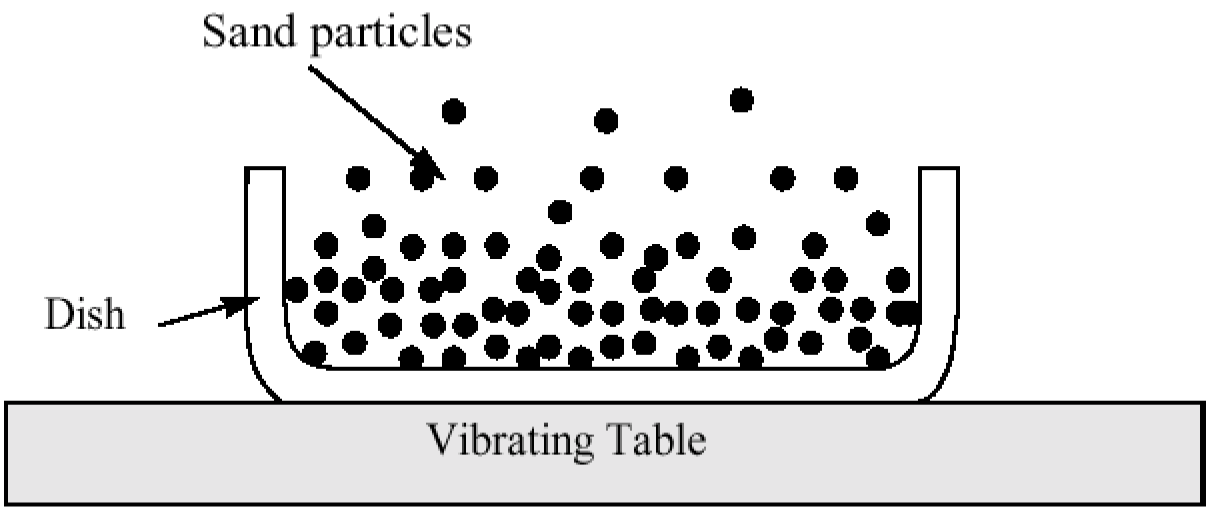
$g_C(E)dE$ = Number of conduction band states/cm^3 lying in the energy range between E and E+dE ($E \geq E_C$)

$g_V(E)dE$ = Number of valence band states/cm^3 lying in the energy range between E and E+dE ($E \leq E_V$)

Note: A state is just an allowable "place" for an electron to sit. It exists whether or not there is an electron in it!

How these states are occupied?

Thermal Equilibrium

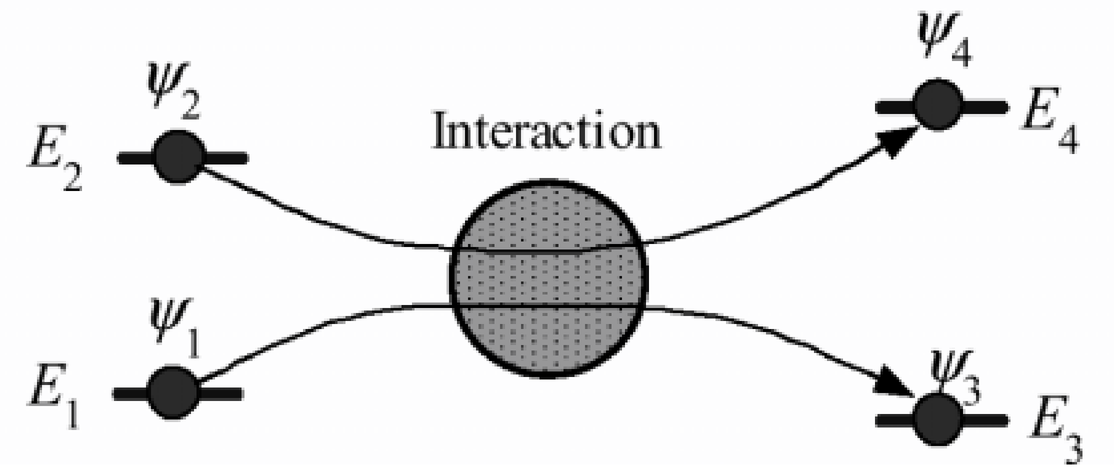


There is a certain probability for the electrons in the conduction band to occupy high-energy states under the agitation of thermal energy (vibrating atoms, etc.)

Boltzman Distribution Function

- Electrons are going to move around energy levels as they collide/ interact with one another.
- Assume a particle like view of electrons:

two electrons at E_1 and E_2 interact to result in electrons at E_3 and E_4



Boltzman Distribution Function

- In steady-state (no net motion of electrons) the probability of going back the other way (E_3 and E_4 interact to result in E_1 and E_2) must be just as likely:
  - $f(E_1)f(E_2)=f(E_3)f(E_4)$
  - Conservation of energy:
    - $E_1+E_2=E_3+E_4$

Solution to the above equations is the **Boltzman distribution function**:

$$f(E)=A\exp(-E/kT)$$

The Fermi Distribution Function

- Boltzmann probability function ignores Pauli's exclusion principle:
  - For an electron to go from E_1 and E_2 to E_3 and E_4, we have to GUARANTEE that E_3 and E_4 are empty!

$f(E_1)f(E_2)[1-f(E_3)][1-f(E_4)] = f(E_3)f(E_4)\,[1-f(E_1)][1-f(E_2)]$

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

The Fermi Function

The Fermi function describes how many of the states at the energy E will be filled with an electron

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

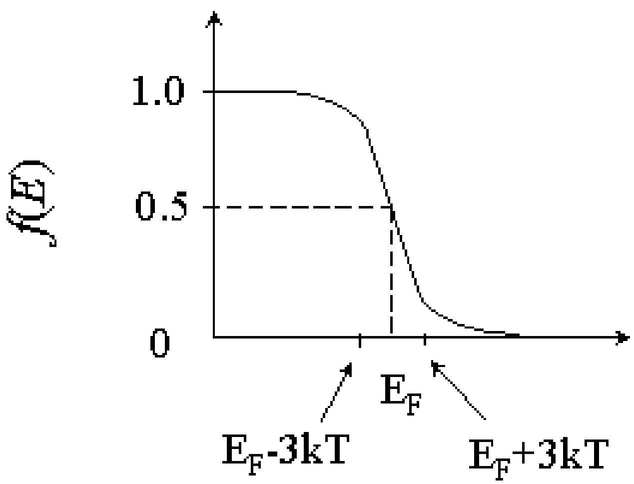
K=Boltzmann constant 8.62×10^{-5} e.V/K, 1.38×10^{-23} J/K.

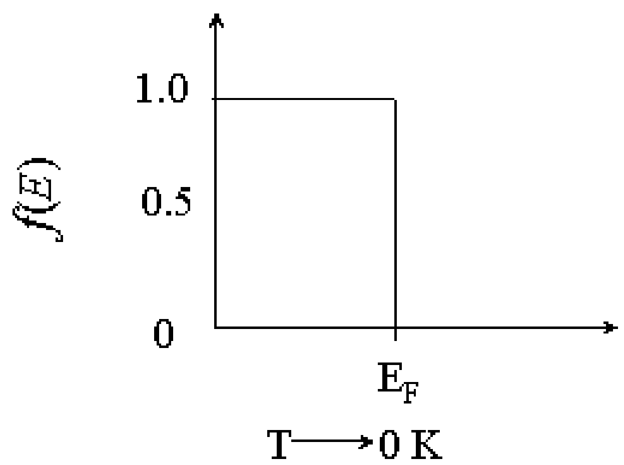
E_F=The Fermi Energy or Fermi Level.

T=Temperature (K).

$f(E)$	Specifies, under equilibrium conditions, the probability that an available state at an energy E will be occupied by an electron
$1 - f(E)$	Specifies, under equilibrium conditions, the probability that an available state at an energy E will not be occupied by an electron

Fermi Energy (Level)



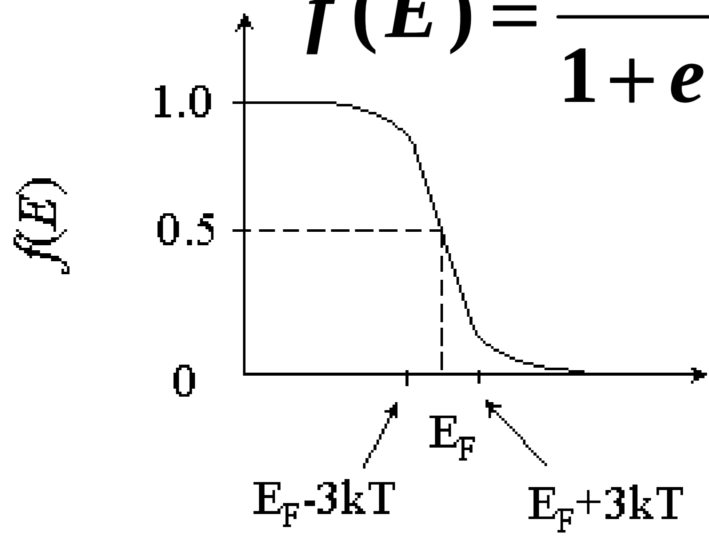


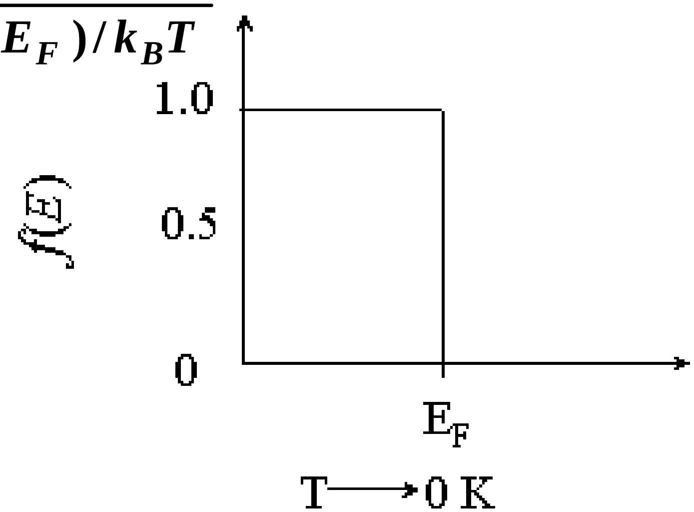
$$f(E) = \frac{1}{1 + e^{(E - E_F)/kT}} \Longrightarrow f(E_f) = \frac{1}{2}$$

E_F is the energy at which exactly one half of states are occupied.

Properties of Fermi Function

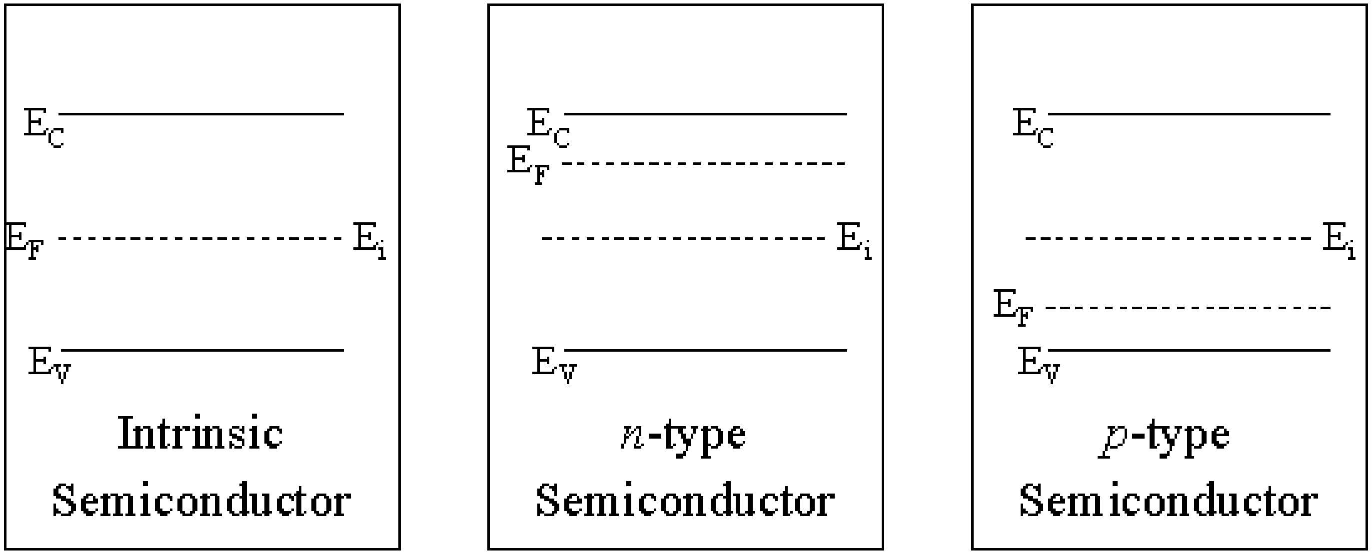
$$f(E) = \frac{1}{1 + e^{(E - E_F)/k_B T}}$$





- if $E >= E_F + 3\,k_B T$,
  - $f(E) \approx \exp(\,(E_F - E)/k_B T\,)$, [<u>Boltzmann distribution</u>]
- if $E <= E_F - 3\,k_B T$,
  - $f(E) \approx 1 - \exp(-\,(E_F - E)/k_B T\,)$

Fermi Level vs. Doping Type in Energy Band Model

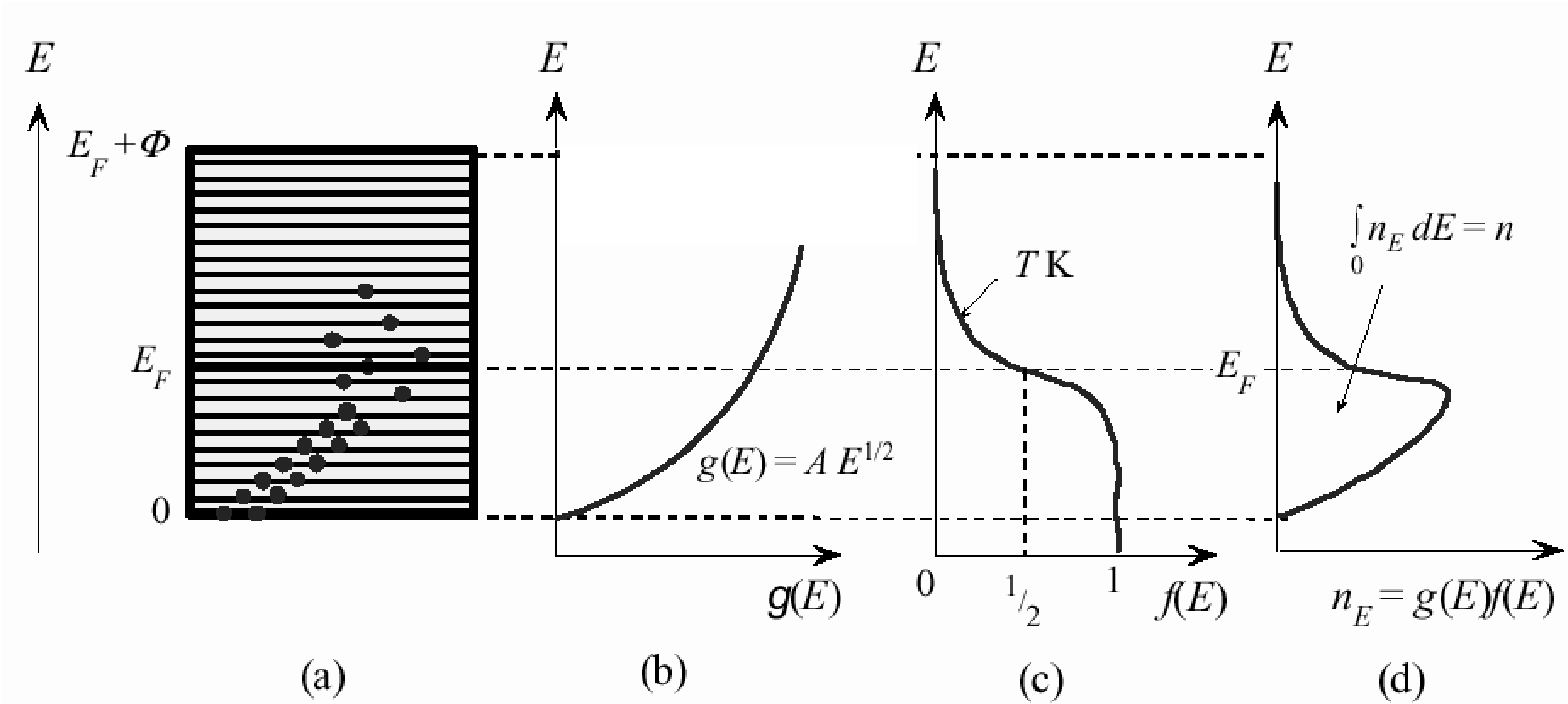


E_i is the intrinsic Fermi level, <u>approximately</u> at the middle of the band gap.

There is only one Fermi-level in a system at equilibrium.

E_F is referenced to E_c, E_v, or E_i

Carrier Concentration



Above 0 K, electrons are excited to higher energy states

DOS vs. E in the band

Probability that a state is occupied at E

The area is the electron concentration.

Formulas for *n* and *p*

$$n \equiv \int_{E_c}^{E_{top}\to\infty} g_c(E) f(E) dE \qquad p \equiv \int_{E_{bot}\to-\infty}^{E_v} g_v(E)(1-f(E)) dE$$

$$n \equiv N_c \frac{2}{\sqrt{\pi}} F_{1/2}\left(\frac{E_F - E_c}{k_B T}\right) \approx N_c e^{(E_F - E_c)/k_B T} \qquad if \quad E_c - E_F \geq 3k_B T$$

$$p \equiv N_v \frac{2}{\sqrt{\pi}} F_{1/2}\left(\frac{E_v - E_F}{k_B T}\right) \approx N_v e^{(E_v - E_F)/k_B T} \qquad if \quad E_F - E_v \geq 3k_B T$$

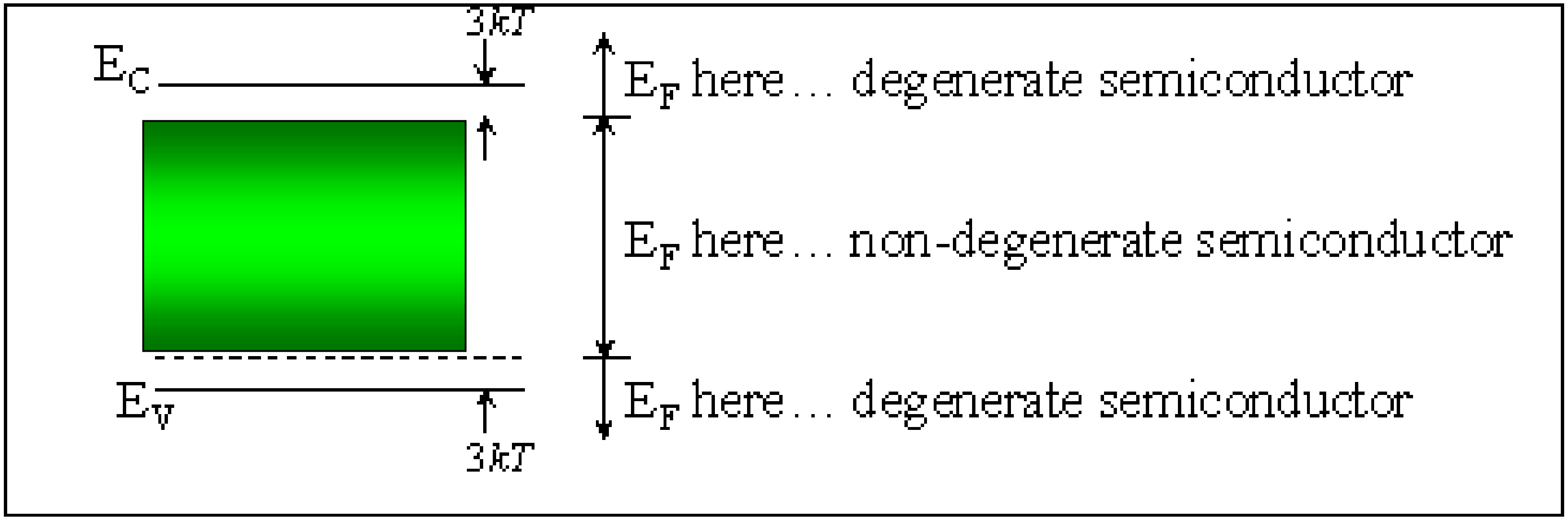
Effective DOS of the Conduction and Valence bands, and Fermi Integral

$$N_c \equiv 2\left(\frac{m_n^* k_B T}{2\pi\hbar^2}\right)^{\frac{3}{2}} \approx 2.51\times10^{19}\left(\frac{m_n^*}{m_0}\right)^{\frac{3}{2}} cm^{-3}$$

$$N_v \equiv 2\left(\frac{m_p^* k_B T}{2\pi\hbar^2}\right)^{\frac{3}{2}} \approx 2.51\times10^{19}\left(\frac{m_p^*}{m_0}\right)^{\frac{3}{2}} cm^{-3}$$

$$F_{1/2}(\eta_c) \equiv \int_0^\infty \frac{\eta^{1/2} d\eta}{1+e^{\eta-\eta_c}}$$

Degenerate vs. Non-Degenerate Semiconductors



- Non-degenerate semiconductor:

  E_F is at least $3k_B T$ below E_C and at least $3k_B T$ above E_V.

Alternative Expression for *n* and *p*

(1)

$$n = N_c e^{(E_F - E_c)/k_B T}$$

$$p = N_v e^{(E_v - E_F)/k_B T}$$

(2) $$n_i = N_c e^{(E_i - E_c)/k_B T} = N_v e^{(E_v - E_i)/k_B T}$$

(3) $$N_c = n_i e^{(E_c - E_i)/k_B T} \quad N_v = n_i e^{(E_i - E_v)/k_B T}$$

(4)

$$n = n_i e^{(E_c - E_i + E_F - E_c)/k_B T} = n_i e^{(E_F - E_i)/k_B T}$$

$$p = n_i e^{(E_i - E_v + E_v - E_F)/k_B T} = n_i e^{(E_i - E_F)/k_B T}$$

Alternative Expression for *n* and *p*

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

$$p = n_i e^{(E_i - E_F)/k_B T}$$

$$np = n_i^2$$

The n_i and the *np* product

$$n_i = N_c e^{(E_i - E_c)/k_B T} = N_v e^{(E_v - E_i)/k_B T}$$

$$n_i^2 = N_c N_v e^{-(E_c - E_v)/k_B T} = N_c N_v e^{-E_g/k_B T}$$

$$\boxed{n_i = \sqrt{N_c N_v}\, e^{-E_g/2k_B T}}$$

Charge Neutrality

For uniformly doped semiconductors:

Charge must be balanced under equilibrium conditons, otherwise charge would flow.

$$\underbrace{qp - qn}_{\text{thermally generated + dopant addition}} \underbrace{- qN_A^- + qN_D^+}_{\text{assumes ionization of all dopant sites}} = 0$$

thermally generated + dopant addition

assumes ionization of all dopant sites

Basic Equations for Carrier Concentration Calculation

- Alternative expression for *n* an *p:*

$$n = n_i \exp\left(\frac{E_F - E_i}{kT}\right)$$

$$p = n_i \exp\left(\frac{E_i - E_F}{kT}\right)$$

- *np* product:

$$np = n_i^{\,2}$$

- Charge neutrality:

$$p - n + N_D - N_A = 0$$

Carrier Concentration Calculation

Charge neutrality: $n + N_a = p + N_d$

$$np = n_i^2$$

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

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

Carrier Concentration Discussion

1) Intrinsic Semiconductor: $n=p=n_i$
2) Doped Semiconductor:

$$\text{if} \quad N_D >> N_A \quad n \cong N_D \quad p \cong \frac{n_i^2}{N_D}$$

$$\text{if} \quad N_A >> N_D \quad p \cong N_A \quad n \cong \frac{n_i^2}{N_A} \quad \text{check} \quad N_D = 10^{16} \quad p \approx 10^4 << n_i$$

3) Doped Semiconductor where $n_i >> |N_A - N_D|$:
   - ➢ All semiconductor become intrinsic at sufficiently high temperatures where $n_i >> |N_A - N_D|$:
4) Compensated Semiconductor:
   - ➢ Both N_A and N_D must be retained in all concentration expressions.

Determination of E_F

$$n_i = N_c e^{(E_i - E_c)/k_B T} = N_v e^{(E_v - E_i)/k_B T}$$

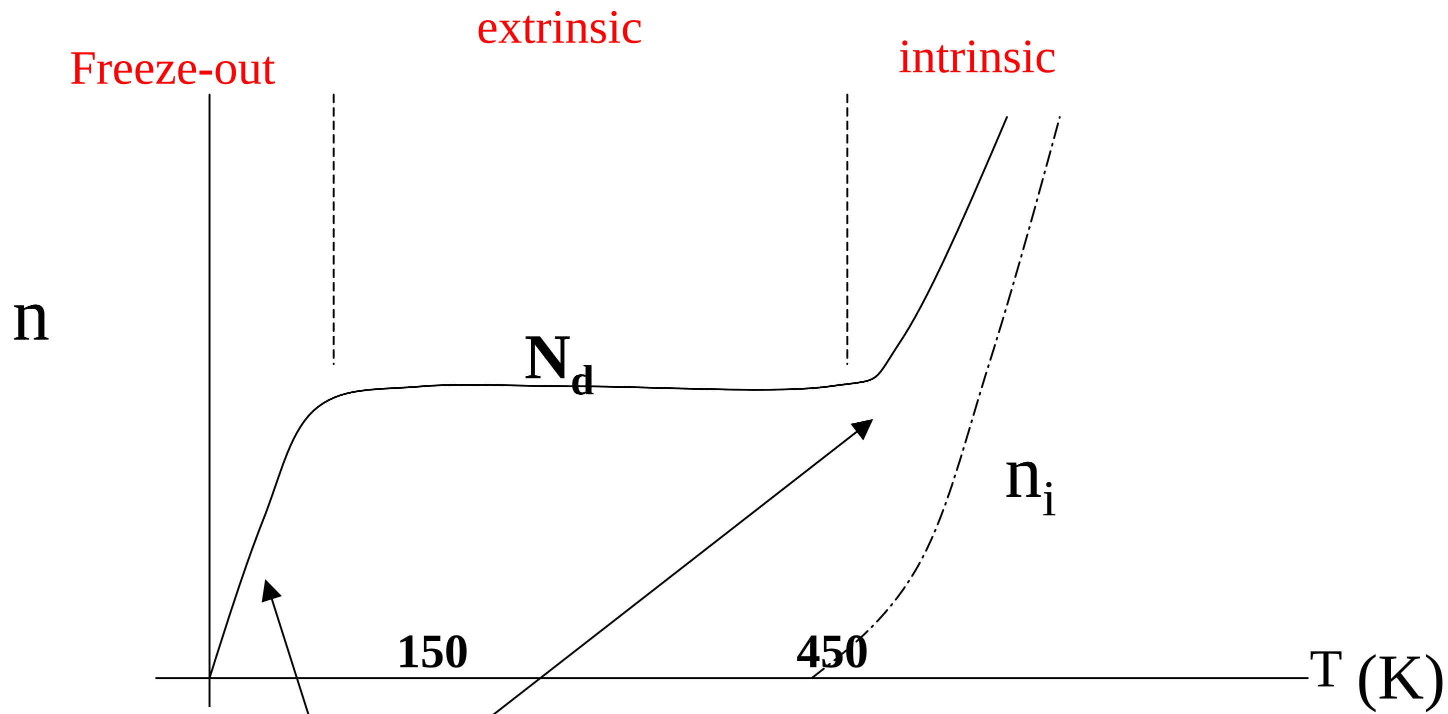
$$\boxed{E_i = \frac{E_c + E_v}{2} + \frac{k_B T}{2}\ln\left(\frac{N_v}{N_c}\right) = \frac{E_c + E_v}{2} + \frac{3k_B T}{4}\ln\left(\frac{m_p^*}{m_n^*}\right)}$$

For a moderately doped semiconductor and complete ionization:

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

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

Temperature Dependence



high T: $n = p = n_i = \sqrt{N_c N_v}\, e^{-E_g/2kT}$

Low T: $n = \left[\frac{N_c N_d}{2}\right]^{1/2} e^{-(E_c - E_d)/2kT}$

To Probe Further

- Reading assignment:
  - Pierrer & Neudeck, Vol. 1, 2.4-2.5.

- References:
  - Streetman, chapter 3
  - Java Applets
    - http://jas2.eng.buffalo.edu/applets/