

ESP5403 Nanomaterials for Energy Systems

Introduction to Semiconductors

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Review of Semiconductor Basics

- Carriers in Semiconductors
- Carrier Concentrations
- Intrinsic & Extrinsic Semiconductors

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Why semiconductors?

- The vast variety of all PV devices on the market today are fabricated from a class of materials known as **semiconductors**. Therefore, we begin the discussion by examining the general nature of semiconducting materials
- Semiconductor meets the important requirement of a photovoltaic material that it has **an energy gap** separating fully occupied states from empty ones.
- **Common semiconductors used for PV Systems:**
 - Crystalline silicon: single (mono) Si - & poly Si
 - Amorphous silicon-hydrogen alloys (a-Si:H)
 - Crystalline gallium arsenide (GaAs)
 - GaAlAs/GaAs heterojunctions
 - Copper sulphide / cadmium sulphide thin films
 - Cadmium Telluride (CdTe)

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What is a semiconductor?

Semiconductors are a group of materials, which have electrical conductivities intermediate between metals (**high conductivity**) and insulators (**low or no conductivity**)

Room temperature conductivities ($\Omega^{-1}\text{m}^{-1}$) of different materials:

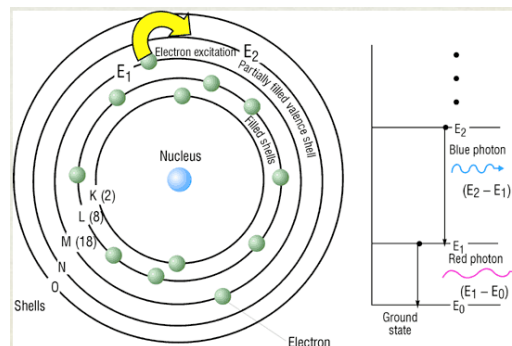
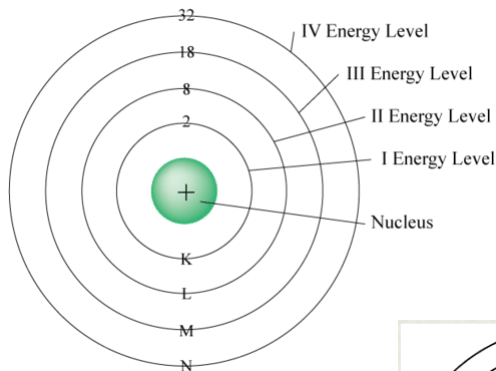
Metals/good metal	Semiconductors	insulators
$10^3 / 10^6$	10^{-3}	10^{-20}

Important feature of semiconductors:

The conductivity of semiconductors can be varied over orders of magnitude by changes in *temperature*, *optical excitation* and *impurity content*. This property makes semiconductor materials natural choice for many electronic devices.

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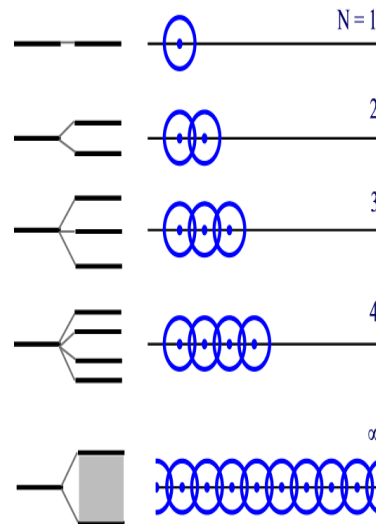


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Energy Levels and Energy Bands

- When far-apart in an isolated atom, the electrons can only have certain distinct energy states
- As atoms come close within proximity of one another, electrons are acted upon (or perturbed) by the electrons and nuclei of adjacent atoms.
- When perturbed, each electron's state may split into a series of closely spaced states, to form what is termed electron energy band.
- The extent of splitting depends on interatomic separation and begins with the outermost electron shells (since they are the first to be perturbed) as the atoms coalesce



Pauli's exclusion principle

No two electrons in an atom can be at the same time in the same state or configuration

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Energy bands

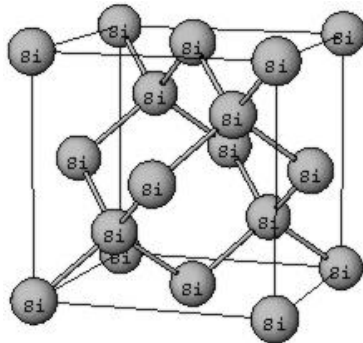
- The electrical properties of solids are a consequence of electron band structure, that is arrangement of the outermost electron bands and the way in which they are filled with electrons.
- The band that contains the highest-energy or Valence Electrons is termed the Valence Band
- The Conduction Band is the next higher energy band, which is under most circumstances, virtually unoccupied by electrons.
- Whether a solid is a conductor, a semi-conductor or an insulator depends on the filling of the valence band and the energy-gap between the valence and the conduction bands

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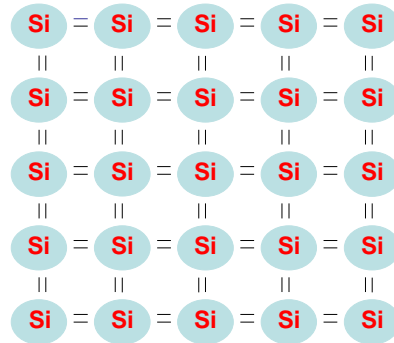
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Si (14) crystal structure

- 3 D view



- 2 D view



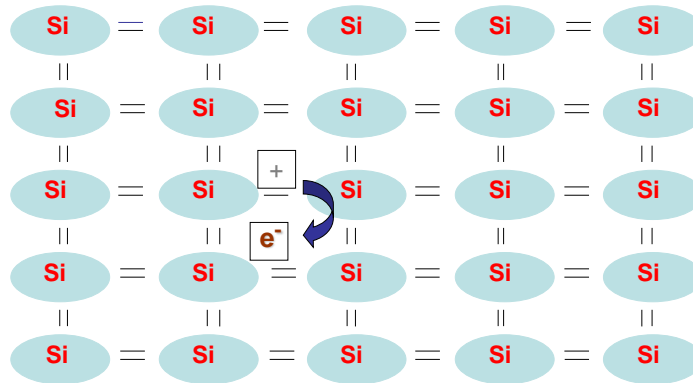
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Carriers : electron & hole

- Carrier is an entity that transports charge from place to place inside a material and hence give rise to electrical current
- Carriers in a semiconductor: **electron and hole**
- Methods of generation of carriers in a semiconductor:
 1. thermal : supplying heat to the system
 2. optical : shining with the light
 3. doping : adding impurities
- Consider Si, at 0 °K, each electron is in its lowest energy state so each covalent bond position is filled.
 => **At 0 °K, silicon is an insulator**
- If a small electric field is applied to the material, no electrons will move because they are bound to their individual atoms.

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Concept of Electron: Bond model



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Concept of electron: Bond model

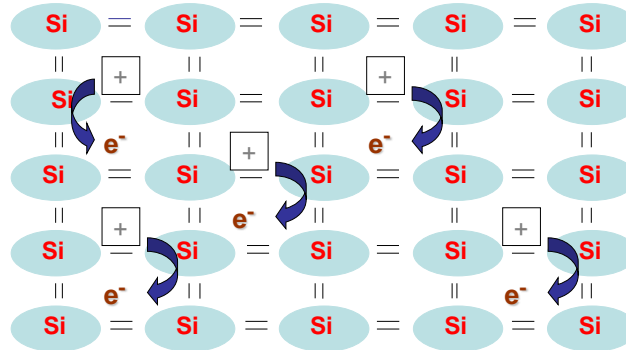
- As temperature increases, the valence electrons gain thermal energy.
- To break a covalent bond, a valence electron must gain a minimum energy E_g , called the energy band gap (number of free electrons is a function of E_g).
- If a valence electron gains enough energy, it may break its covalent bond and move away from its original position.
- This electron is free to move within the crystal.

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Concept of hole : Bond model

- As temperature increases, more bonds are broken creating more negative free electrons and more positively charged empty states (number of free electrons is a function of temperature.)

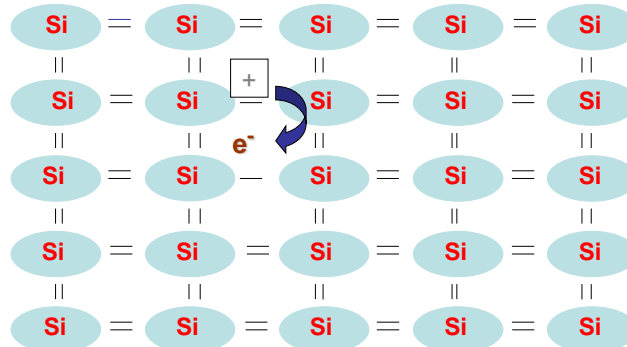


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Concept of Hole: Bond model

- Since the net charge of a crystal is zero (charge neutrality), if a negatively (-) charged electron breaks its bond and moves away from its original position, a positively charged “empty state” is left in its original position

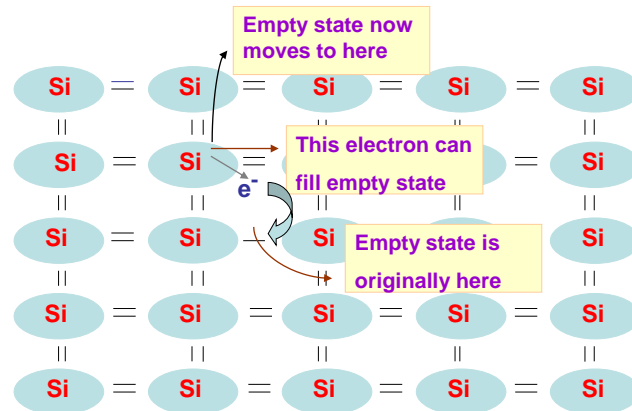


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Concept of Hole: Bond model

An electron in the neighborhood, that has sufficient energy and is adjacent to an empty state may move into the empty state, leaving an empty state behind



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Concept of Hole: Bond model

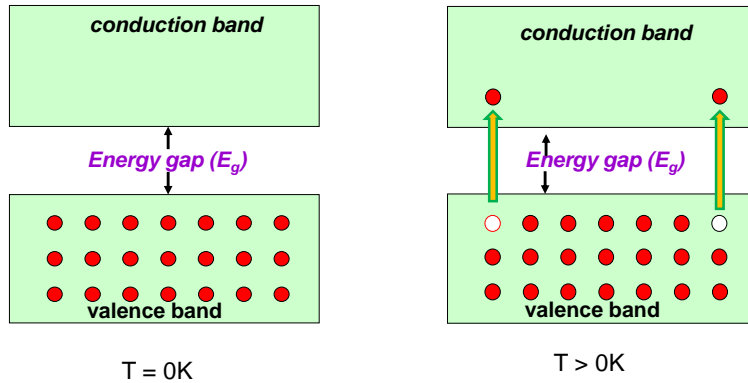


- As another electron moves into the space, it leaves another hole behind it, etc
- Moving empty states can give the appearance that positive charges move through the material.
- This moving empty state is modeled as a positively charged particle called a hole.
- Movement of electron into the “empty state” \equiv movement of ‘empty state’ i.e. the “hole” itself. Therefore, the directions of motion of an electron and hole are opposite to each other
- In semiconductors, two types of “particles” contribute to the current: positively charged holes and negatively charged electrons

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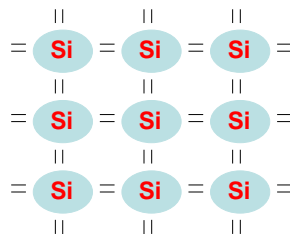
Concept of electron and hole: *Band Model*



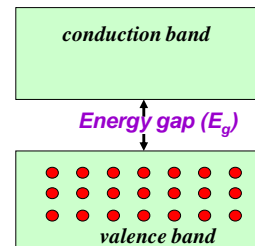
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Comparison of bond model with band model

At $T = 0\text{K}$



No bonds broken



Conduction band is empty

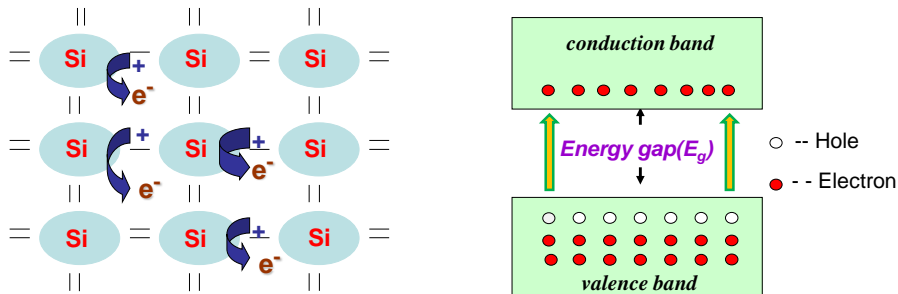
➤ No carriers ➡ insulator

➤ Energy required to break a covalent bond is equivalent to the bandgap E_g

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Comparison of bond model with band model

At $T = 300K$



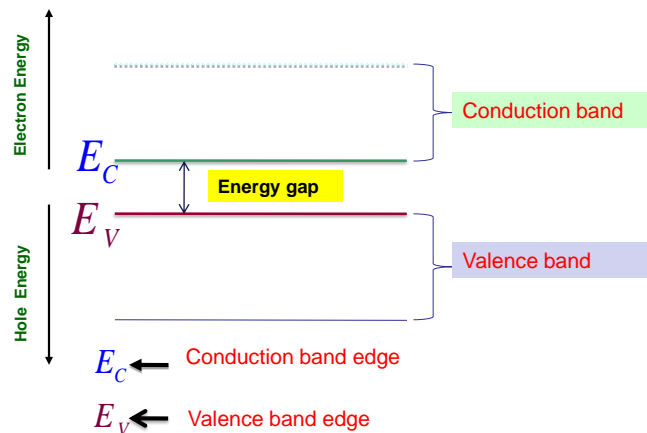
Electron excited into CB is now mobile as there are unoccupied states available.

Available state in VB now allows successive electron movement in VB. Seen as the motion of a hole in the VB.

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Energy diagram: basic definitions



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Energy diagram: basic definitions

- The *conduction band edge*, E_c **is the lowest energy level in the conduction** band. Electrons in the C.B. normally reside at energy levels around E_c as these are the lowest energy states in the C.B.
- The *valence band edge*, E_v **is the highest electron energy level in the** valence band. Holes in the VB normally reside at energy levels around E_v as these are the lowest energy states for holes in the VB.
- The *band gap* $E_g = E_c - E_v$, **is the minimum energy required to create an electron-hole pair (EHP)**. Note that *thermal excitation across the band gap* always creates electrons and holes in pairs

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Energy diagram: basic definitions

- By convention, energy band diagrams are energy diagrams for negatively charged electrons, with energy increasing from bottom to top
- For electrons in the C.B, the lowest energy states are at the bottom of the C.B, and hence electrons tend to stay in these low energy states near E_c
- For holes, which are positively charged, their energy increases from the top of a band to the bottom of a band
- Holes in the V.B are found in the lower-energy states for holes, which are at the top of the V.B. E_v

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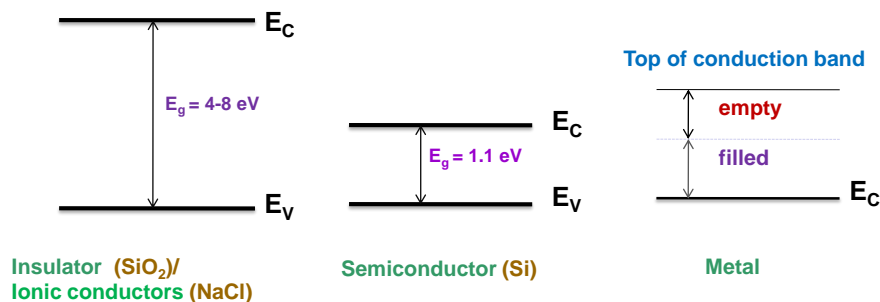
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Carrier Properties: Charge

- Charge of electron = $-e = -1.602 \times 10^{-19} \text{ C}$
- Charge of hole = $+e = +1.602 \times 10^{-19} \text{ C}$

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Insulators/Ionic conductors, Semiconductors, and Metals



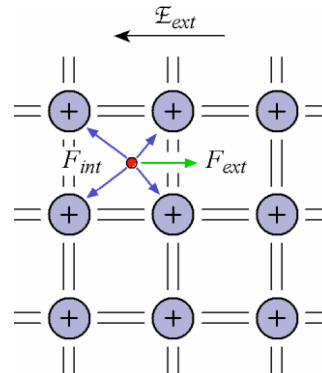
- Metals conduction band is half filled
- Semiconductors have lower E_g than insulators and can be doped.
- Totally filled bands and totally unfilled bands do not allow current flow, no free electrons because they are all taking part in interatomic bonds.

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Carrier Properties: Effective Mass

Consider electrons first.

Electrons in CB are not entirely “free” as they are travelling in the background potential of the lattice atoms (nuclei, electron shells)



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Carrier Properties: Effective Mass

- Electrons experience internal forces F_{int} due to the background potential of the lattice atoms.
- When an external force F_{ext} (e.g. an electric field) is applied to the conduction electrons, the equation of motion for the electrons can be written as:

$$F_{int} + F_{ext} = m_0 a \quad (2.1)$$

where, m_0 = free electron mass (9.108×10^{-31} kg)

a = acceleration

- **Internal and external forces act on a conduction electron**

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Carrier Properties: Effective Mass

- To treat the electrons as if they were truly free particles that respond to the external force (only), we wish to hide the internal force term in the equation of motion.

- We can re-write the equation of motion as: $F_{ext} = m_e^* a$ (2.2)

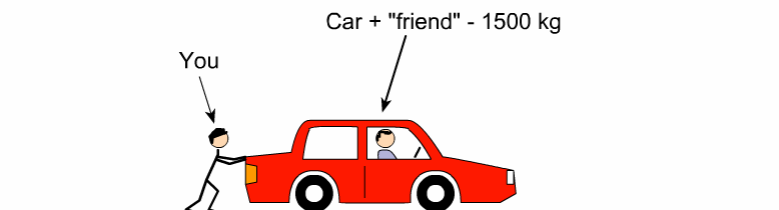
where m_e^* is the effective mass of an electron in the CB.

- The effective mass now includes and takes care of the effects of the internal lattice forces on the electron.
- Electrons residing near the bottom of the CB behave like free electrons, but with an effective mass given by m_e^*

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Carrier Properties: Effective Mass – An analogy

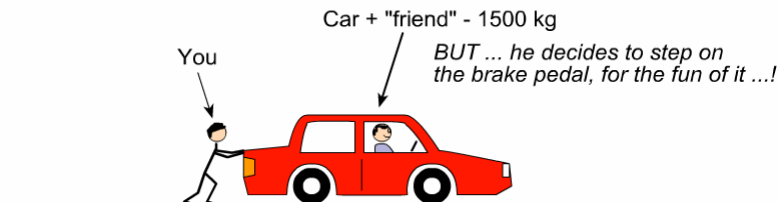


Motion of car is governed by the force you exert (the external force), and the true mass of the car.

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Carrier Properties: Effective Mass – An analogy



The internal forces (the applied brakes) opposes your exerted force and makes the car “feel” heavier to you. It has a larger effective mass, as far as you are concerned. For the same external force, the car accelerates slowly

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Carrier Properties: Effective Mass – An analogy



The internal forces (the engine) assists your exerted force and makes the car “feel” lighter to you. It has a smaller effective mass, as far as you are concerned. For the same external force, the car accelerates more.

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Effective mass for holes

- Motion of holes at the top of the VB results from the collective effects produced by electrons moving in a nearly full band.
- The motion of a hole is thus also affected by the internal lattice forces.

$$F_{ext} = m_h^* a \quad (2.3)$$

where m_h^* is the effective mass of a hole.

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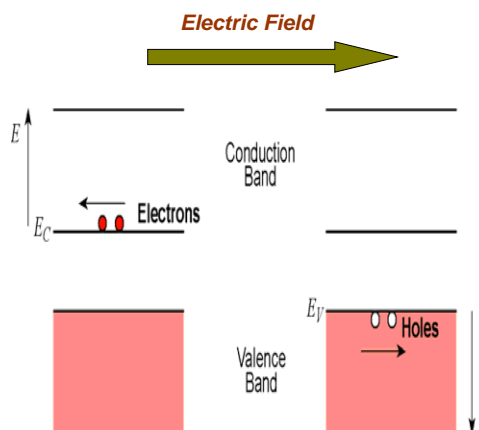
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Carrier properties: Carrier motion in electric field

- Under the influence of an external electric field, holes move in the opposite direction to electrons.

- Currents are in the same direction (due to opposite charge)

- Note that the energy for holes increase from the top of the VB to the bottom of the VB.



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Review of Semiconductor Basics

- Carriers in Semiconductors
- **Carrier Concentrations**
- Intrinsic & Extrinsic Semiconductors

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Carrier Concentrations/densities

- The concentrations of holes and free electrons are important quantities in the behavior of semiconductors
- Carrier concentration is given as the number of carriers per unit volume, or

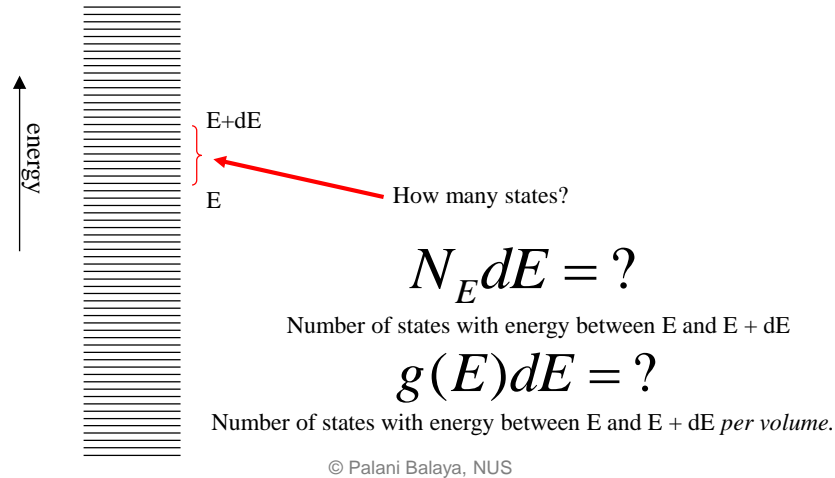
Carrier concentration = # / cm³

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(i) Density of states

In a semiconductor the number of energy levels is very large and are very close together



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Density of states.....

In general,

$$g(E) dE = \frac{8\sqrt{2}\pi m^{3/2}}{h^3} \cdot E^{1/2} dE \quad (2.4)$$

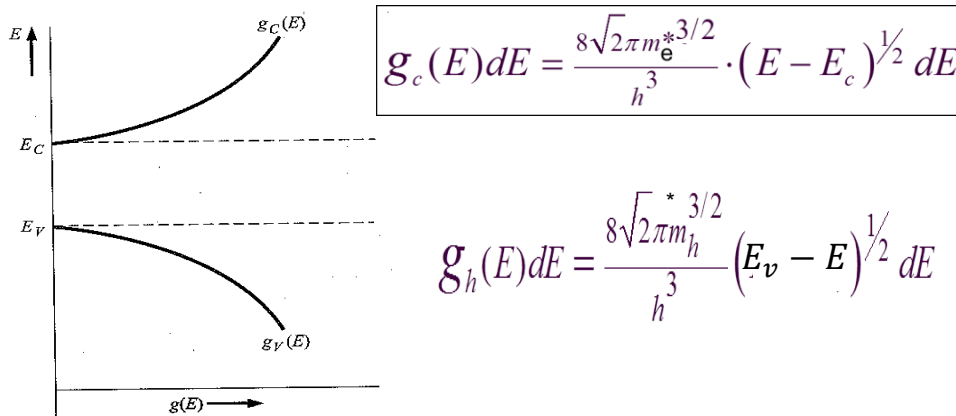
For an electron in a Conduction Band

$$g_c(E) dE = \frac{8\sqrt{2}\pi m_e^{3/2}}{h^3} \cdot (E - E_c)^{1/2} dE \quad (2.5)$$

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Density of states.....



Density of states in the CB and density of states in the VB as a function of energy

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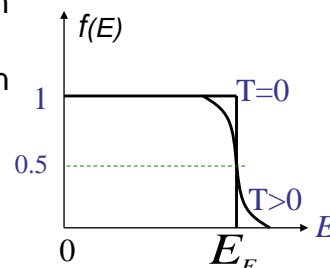
(ii) Fermi Function

At finite temperature the probability that an electron can occupy a particular energy level E is given by Fermi Dirac distribution function:

$$f(E) = \frac{1}{1 + \exp\left[-\frac{E - E_F}{kT}\right]} \quad (2.6)$$

where:

E_F = Fermi energy or Fermi level energy for which occupation probability is 50%



Fermi function as a function of energy at a temperature

$$k = \text{Boltzmann constant} = 8.62 \times 10^{-5} \text{ eV/K} \\ = 1.380649 \times 10^{-23} \text{ J/K}$$

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Fermi energy or Fermi level

The Fermi energy is the highest occupied level at absolute zero.

At absolute zero there is no thermal energy, so electrons fill the band starting from the bottom and there is a sharp cutoff at the highest occupied energy level. This energy defines the Fermi energy.

At finite temperatures there is no sharply defined most energetic electron because thermal energy is continuously exciting electrons within the band. The best you can do is define the energy level with a 50% probability of occupation, and this is the Fermi level.

The Fermi level is the same as chemical potential (or one should say "electrochemical potential"), i.e. the energy at which a state has 50% chance of being occupied, while the Fermi energy is the Fermi level at absolute zero.

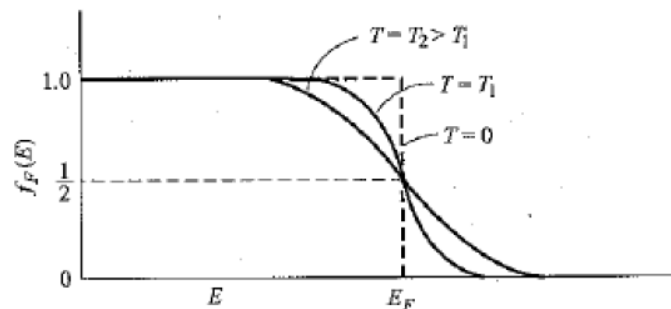
In short:

- Fermi level is the chemical potential. It is the energy level with 50% chance of being occupied at finite temperature T .
- Fermi energy does not depend on temperature.
- Fermi level does depend on temperature.

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Fermi function with temperature



At room temperature (300 K), $kT = 0.026$ eV and $3kT = 0.078$ eV $\ll E_G$ (Si).

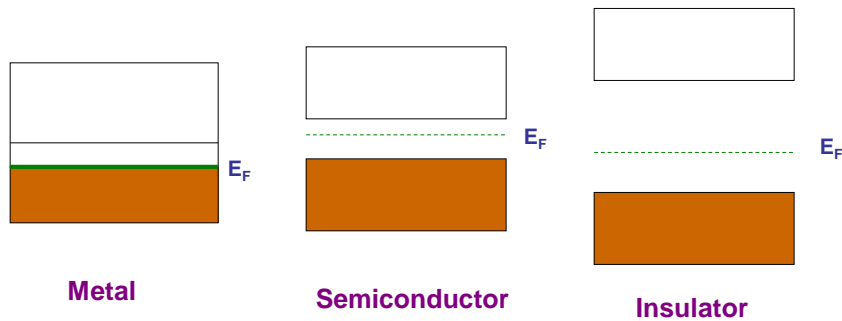
Compared to Si band gap, $3kT$ energy interval that appears prominently in the $T > 0$ K formalism is typically quite small.

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Fermi Function.....

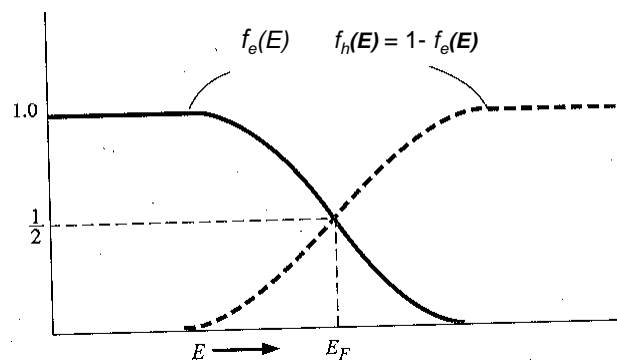
The Fermi function is completely general, and applies to any solid material in thermal equilibrium.



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Fermi Function.....



The probability of a state being occupied, $f_e(E)$, and the probability of a state being empty, $f_h(E) = 1 - f_e(E)$

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Carrier Concentrations at Equilibrium

Density of electrons in C.B.

First we deal with the electrons in CB.....

The density of occupied states per unit volume and unit energy, $n(E)$, is simply the product of the density of states in the conduction band, $g_c(E)$ and the Fermi-Dirac probability function, $f_e(E)$ (also called the Fermi function)

$$n(E) = g_c(E) f_e(E) \quad (2.7)$$

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Density of electrons in C.B.....

The number of electrons per unit volume in the range from E to $E+dE$

$$dn = g_c(E) f_e(E) dE \quad (2.8)$$

The carrier density, is obtained by integrating the product of the density of states and the probability density function over all possible states

For electrons in the conduction band the integral is taken from the bottom of the conduction band, labeled, E_c , to the top of the conduction band (generally , ∞)

$$n_0 = \int_{E_c}^{\infty} g_c(E) f_e(E) dE \quad (2.9)$$

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Density of electrons in C.B.....

$g_c(E)dE$, is density of states in the conduction band

$$g_c(E) = \frac{8\sqrt{2}\pi m_e^{3/2}}{h^3} \cdot (E - E_c)^{1/2} \quad (2.10)$$

where:

m_e^* = effective mass of electrons,

E_c = energy of conduction band edge

$h = 6.626 \times 10^{-34} \text{ m}^2 \text{ kg / s}$; Planck Constant

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Density of electrons in C.B.....

Further we assume that:

1. Fermi level is within the forbidden energy band gap (at mid gap)
2. For electrons in the C.B, we have $E > E_c$

If $(E_c - E_F) \gg kT$, then $(E - E_F) \gg kT$,

$k = 8.617 \times 10^{-5} \text{ eV K}^{-1}$; Boltzmann Constant

$$f_e(E) = \frac{1}{1 + e^{(E - E_F) / kT}} \approx \exp\left[-\frac{E - E_F}{kT}\right] \quad (2.11)$$

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Density of electrons in C.B.....

substituting eq. 2.10 and 2.11 in eq.2.9,we get,

$$n_0 = \frac{8\sqrt{2}\pi m_e^{*3/2}}{h^3} \int_{E_c}^{\infty} (E - E_c)^{1/2} \exp\left[-\frac{(E - E_F)}{kT}\right] dE$$

$$n_0 = \frac{8\sqrt{2}\pi m_e^{*3/2}}{h^3} \exp\left[-\frac{E_c - E_F}{kT}\right] \int_{E_c}^{\infty} (E - E_c)^{1/2} \exp\left[-\frac{E - E_c}{kT}\right] dE$$

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Density of electrons in C.B.....

put $\frac{E - E_c}{kT} = x$, then $dE = kT dx$

$$n_0 = \frac{8\sqrt{2}\pi m_e^{*3/2}}{h^3} \exp\left[-\frac{E_c - E_F}{kT}\right] \int_0^{\infty} x^{1/2} e^{-x} dx (kT)^{3/2} \quad (2.12)$$

Using, $\int_0^{\infty} x^{1/2} e^{-x} dx = \sqrt{\pi}/2$

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Density of electrons in C.B.....

$$n_0 = 2 \left(\frac{2\pi m_e^* kT}{h^2} \right)^{3/2} \exp \left[-\frac{E_c - E_F}{kT} \right] \quad (2.13)$$

$$n_0 = N_C \exp \left[-\frac{E_c - E_F}{kT} \right] \quad (2.14)$$

where $N_C = 2 \left(\frac{2\pi m_e^* kT}{h^2} \right)^{3/2}$

known as effective density of states for electrons

In Si,

$$N_C = 2.51 \times 10^{19} (m_e^*/m_0)^{3/2} \text{ cm}^{-3} = 2.8 \times 10^{19} \text{ cm}^{-3}$$

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1.2.3.(b). Density of holes in V.B.

Similarly, the concentration of free holes (P_0) in the valence band is

$$P_0 = \int_{-\infty}^{E_v} g_h(E) f_h(E) dE \quad (2.15)$$

$$g_h(E) dE = \frac{8\sqrt{2}\pi m_h^*{}^{3/2}}{h^3} (E_v - E)^{1/2} dE \quad (2.16)$$

$$f_h(E) = 1 - f_e(E) = 1 - \left(\frac{1}{1 + e^{(E - E_F)/kT}} \right) \approx e^{-(E_F - E)/kT} \quad (2.17)$$

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Density of holes in V.B.....

In the V.B., $E < E_V$ or $E < E_F$ or $E_F - E_V \gg kT$ (2.18)

Using similar approach as above,

$$p_0 = N_V \exp\left[-\frac{E_F - E_V}{kT}\right] \quad (2.19)$$

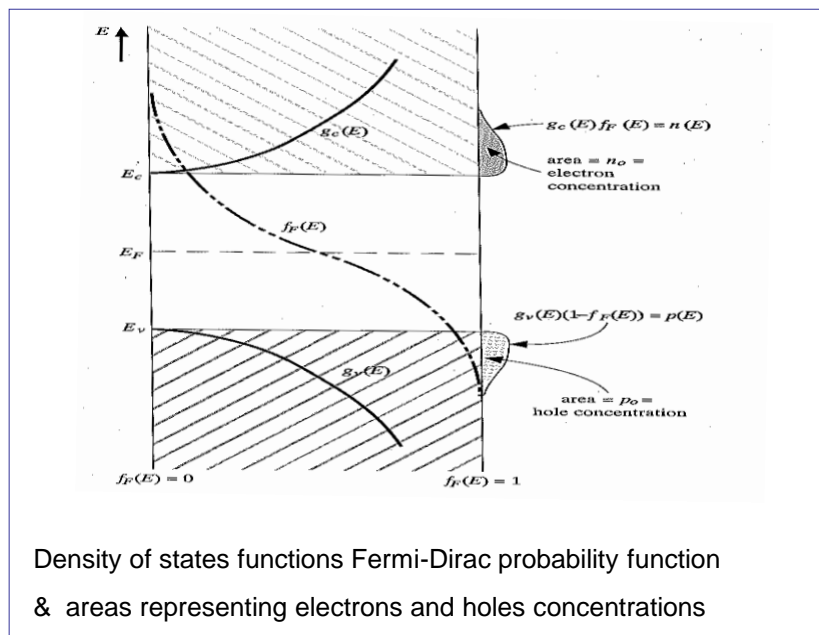
where, $N_V = 2 \left(\frac{2\pi m_h^* kT}{h^2} \right)^{3/2}$

known as effective density of V.B. states

In Si,

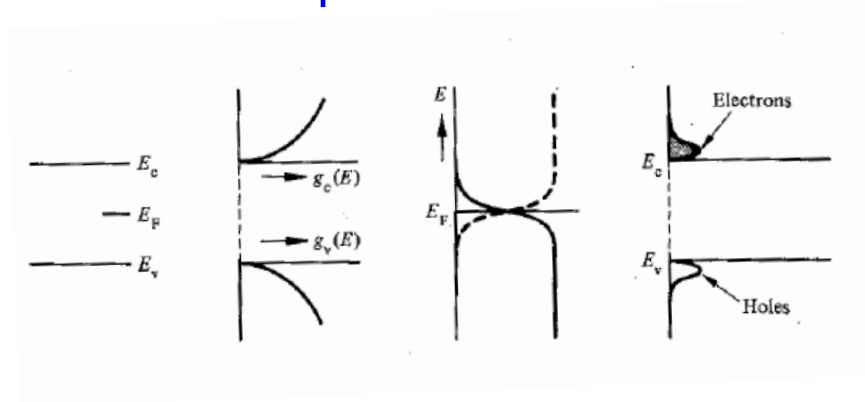
$$N_V = 2.51 \times 10^{19} (m_h^*/m_0)^{3/2} \text{ cm}^{-3} = 1.0 \times 10^{19} \text{ cm}^{-3}$$

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Carrier distribution in their respective bands



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Review of Semiconductor Basics

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- Carrier Concentrations
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Intrinsic Carrier Concentrations

Intrinsic semiconductor:

- In an intrinsic semiconductor, **the number of holes and free electrons are the same**
- If an electron breaks its covalent bond we have one free electron and one hole
- n_i = *the concentration of free electrons in an intrinsic semiconductor.*
= the concentration of holes in an intrinsic semiconductor.

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Intrinsic Carrier Concentrations

What do you get when you multiply n_o with p_o ?

- The result gives an intrinsic property of the semiconductor
- This property is referred to as the **mass action law**. It is a powerful relation, which enables to quickly find the hole density if the electron density is known or vice versa. This relation is only valid for non-degenerate semiconductors in thermal equilibrium (Two or more different states of a quantum mechanical system are said to be **degenerate** if they give the same value of energy upon measurement)
- It turns out that the product of the electron and hole density, in a non-degenerate semiconductor is always equal to the square of the intrinsic carrier density, and this is true not only for intrinsic semiconductors

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Intrinsic carrier concentration

In an intrinsic semiconductor, we have

$$n_0 = p_0 = n_i$$

By writing, E_i for E_F we can then write two relations between the intrinsic carrier density at the intrinsic Fermi energy

$$n_i = n_0|_{(E_F=E_i)} = N_c \exp\left(-\frac{E_c - E_i}{kT}\right) \quad (2.20)$$

$$n_i = p_0|_{(E_F=E_i)} = N_v \exp\left(-\frac{E_i - E_v}{kT}\right) \quad (2.21)$$

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Intrinsic carrier concentration

multiplying eq. s 2.20 & 2.21, we get

$$n_i^2 = n_0 p_0 = N_c N_v \exp\left[-\frac{E_c - E_v}{kT}\right] = N_c N_v \exp\left(-\frac{E_g}{kT}\right)$$

$$n_i = (N_c N_v)^{1/2} \exp\left(-\frac{E_g}{2 kT}\right) \quad (2.22)$$

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Intrinsic Fermi energy

The above equations for the intrinsic electron and hole density can be solved for the intrinsic Fermi energy ($E_i = E_F$) by taking the ratio of equations 2.20 & 2.21 yielding:

$$E_i = \frac{E_c + E_v}{2} + \frac{1}{2} kT \ln \left(\frac{N_v}{N_c} \right) \quad (2.23)$$

using N_c and N_v values,

$$E_i = \frac{E_c + E_v}{2} + \frac{3}{4} kT \ln \left(\frac{m_h^*}{m_e^*} \right) \quad (2.24)$$

The intrinsic Fermi energy is typically close to the **midgap** energy, half way between the conduction and valence band edge

$$n_i = n_0|_{(E_F=E_i)} = N_c \exp \left(-\frac{E_c - E_F}{kT} \right) \quad n_i = p_0|_{(E_F=E_i)} = N_v \exp \left(-\frac{E_F - E_v}{kT} \right)$$

Intrinsic material as reference

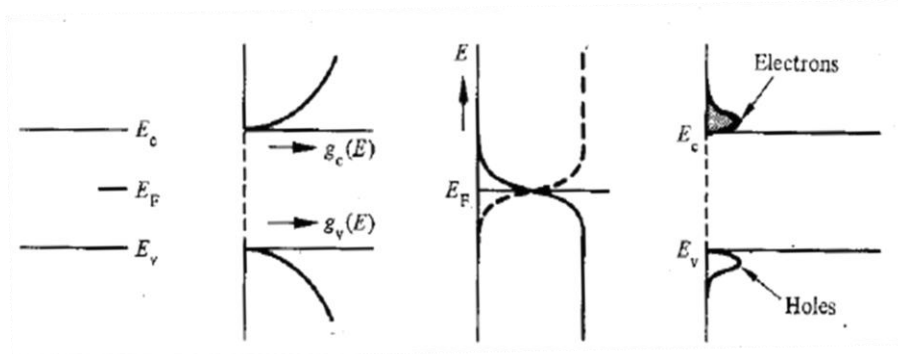
Dividing the expressions for the carrier densities 2.14 & 2.19, by those for the intrinsic density 2.20 & 2.21 allows to write the carrier densities as a function of the intrinsic carrier density and the intrinsic Fermi energy:

$$n_0 = n_i \exp \left(\frac{E_F - E_i}{kT} \right) \quad (2.25)$$

$$p_0 = n_i \exp \left(\frac{E_i - E_F}{kT} \right) \quad (2.26)$$

We will use primarily these two equations to find the electron and hole density in a semiconductor in thermal equilibrium

Determination of E_F (intrinsic semiconductor) Fermi energy at bandgap



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Intrinsic Fermi energy- practical case of Si

E_i lies precisely at midgap only if $m_h^* = m_e^*$ or if $T = 0$ K.

In reality, for more practical case of Si at room temperature, $m_h^* / m_e^* = 0.69 - 0.75$ (considering the density of states calculation), and hence

$$\left(\frac{3}{4}\right) kT \ln\left(\frac{m_h^*}{m_e^*}\right) = -0.0073 \text{ eV}$$

E_i lies 0.0073 eV below midgap.

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Intrinsic Fermi energy

Intrinsic Fermi level above the center of the bandgap

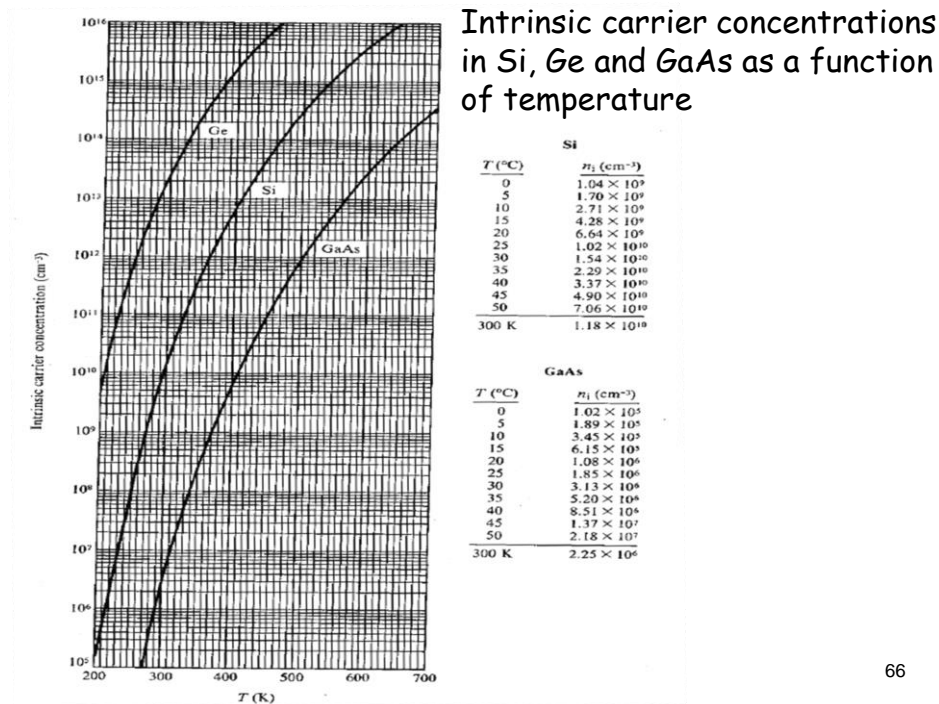
If $m_h^* > m_e^*$, then $E_i > E_{midgap}$

Intrinsic Fermi level below the center of the bandgap

$m_h^* < m_e^*$ $E_i < E_{midgap}$

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Charge neutrality relationship

- Charge neutrality relation provides the general tie between carrier and dopant concentration
- Consider a uniformly doped semiconductor: dopant atoms/cm³ is same everywhere
- Examine every little section of semiconductor; assume equilibrium conditions, one notices no net charge
- If not, local electric field exists giving rise to carrier motion-associated current - totally inconsistent with equilibrium condition

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Charge neutrality relationship

Electrons, holes, ionized donor sites, ionized acceptor sites – all exist in semiconductor

For uniformly doped semiconductor – charge neutrality requires **(note $n = n_o$ and $p = p_o$)**

$$\frac{\text{charge}}{\text{cm}^3} = qp - qn + qN_D^+ - qN_A^- = 0$$

$$p - n + N_D^+ - N_A^- = 0 \quad (2.27)$$

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Charge neutrality relationship

By definition,

N_D^+ = number of ionized (positive charged) donor site/cm³

N_A^- = number of ionized (negatively charged) acceptor sites/cm³

At room temperature there is sufficient thermal energy available in a semiconductor to ionize almost all of the shallow-level donor and acceptor sites.

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Charge neutrality relationship

Defining,

N_D = total number of donor atoms or sites/cm³

N_A = total number of acceptor atoms or sites/cm³

and setting,

$$N_D^+ = N_D$$

$$N_A^- = N_A$$

One obtains: $p - n + N_D - N_A = 0$ (2.28)

Standard form of charge neutrality relationship

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Extrinsic semiconductors

Since concentration of free electrons and holes is small, only very small currents are possible.

Impurities can be added to semiconductors to increase the concentration of free electrons and holes.

Addition of impurities is called doping and added impurities is known as dopants. And the resultant semiconductor is extrinsic semiconductor.

Extrinsic semiconductors are extensively used in the fabrication of various semiconductor devices including solar cells.

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Extrinsic semiconductors

An impurity would have one less or one more electron in the valence shell than silicon.

Impurities for group 4 type atoms (silicon) would come from group 3 or group 5 elements. The common dopants are listed below:

Group V		Group III	
P [*]	} <i>n</i> -type	B [*]	} <i>p</i> -type
As			
Sb			
		Ga	
		In	
		Al	

* most widely employed dopants

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n -type Extrinsic semiconductor

The most common group V elements are **P** and **As**

Group V elements have 5 electrons in valence shell

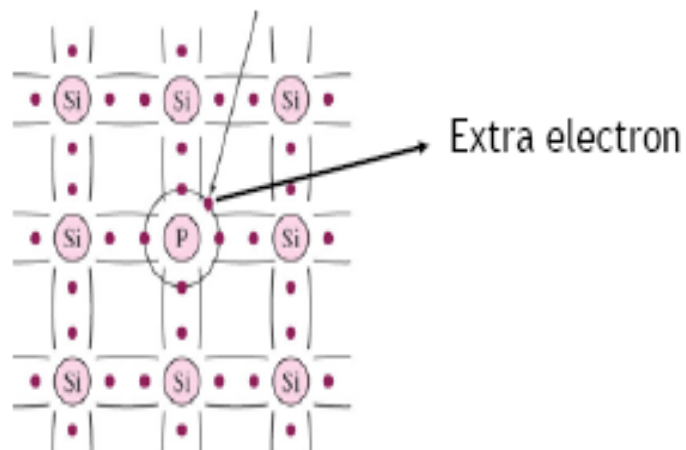
Four of the electrons fill the covalent bond in Si crystal structure

The 5th electron is loosely bound to the impurity atom and is a free electron at room temperature, thus acts as a carrier

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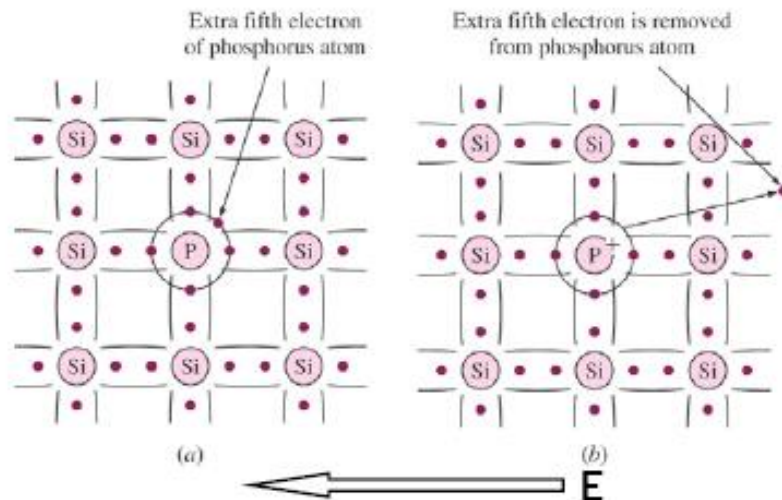
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n -type Extrinsic semiconductor



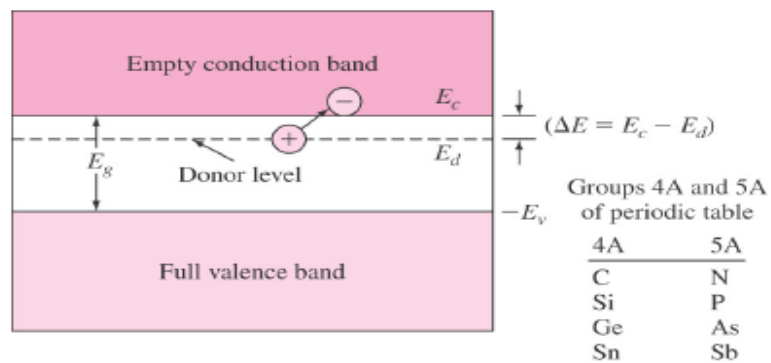
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n-type Extrinsic semiconductor



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n-type extrinsic semiconductor: Energy level diagram



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***n*-type Extrinsic semiconductor**

The group 5 atom is called a **donor** impurity since it donates a free electron.

The group 5 atom has a net positive charge that is fixed in the crystal lattice and cannot move.

With a donor impurity, free electrons are created without adding holes.

A semiconductor doped with donor impurities has excess free electron and is called an ***n*-type** semiconductor.

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***P*-type Extrinsic semiconductor**

The most common group 3 impurity is boron which has 3 valence electrons

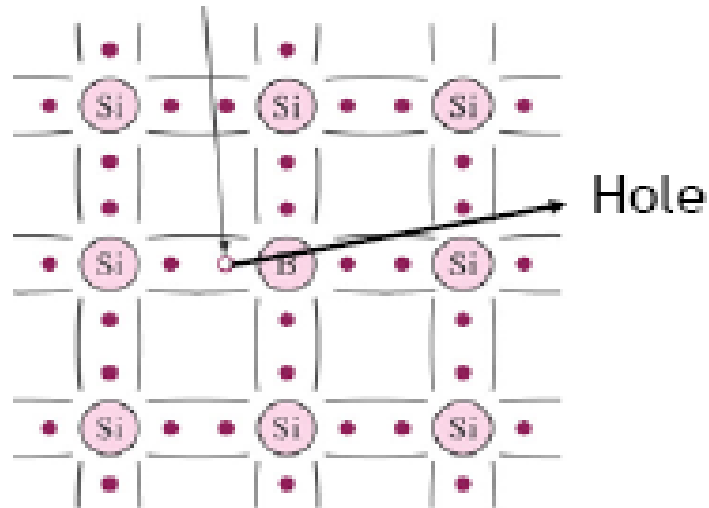
Since boron has only 3 valence electrons, the boron atom can only bond with three of its neighbors leaving one open bond position

At room temperature, silicon has free electrons that will fill the open bond position, creating a hole in the silicon atom from where it came.

The boron atom has a net negative charge because of the extra electron, but the boron atom cannot move.

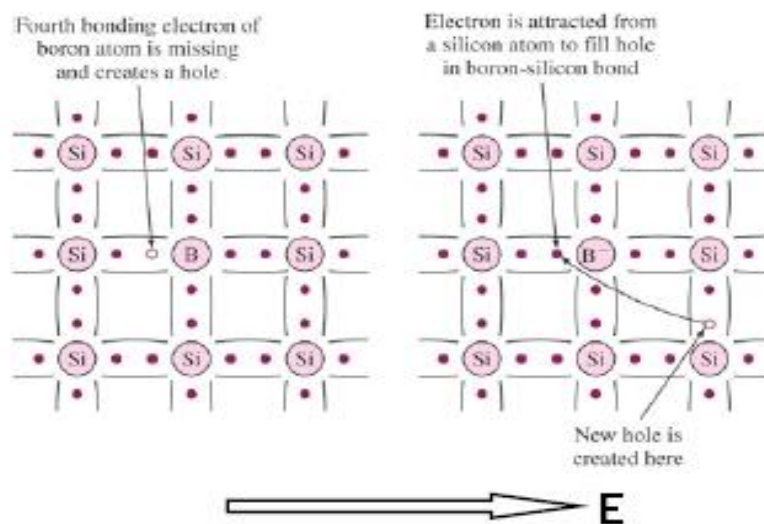
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P-type Extrinsic semiconductor



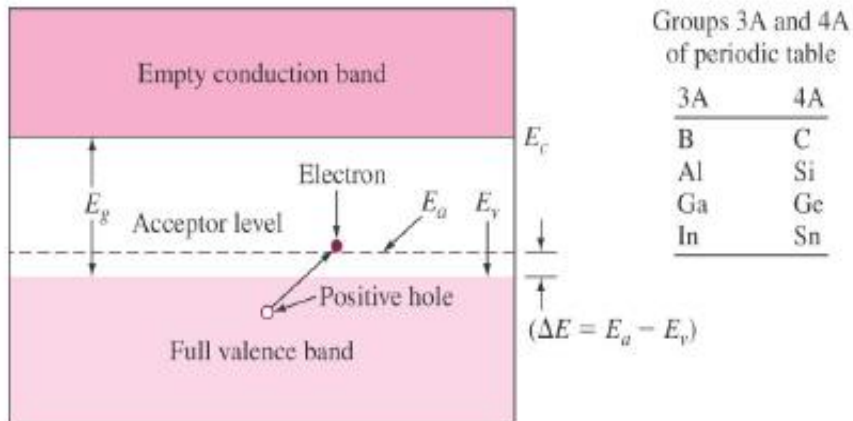
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P-type Extrinsic semiconductor



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P-type Extrinsic semiconductor: Energy Level diagram



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Carrier concentration calculations

Let us calculate carrier concentration in doped semiconductor under equilibrium conditions

Assumptions:

1. Non-degeneracy (allowing us to use np product relationship)
2. Total ionization of dopant sites
3. n_i that appears in $n_o p_o$ product expression, has been calculated and plotted – known quantity
4. N_A and N_D are typically controlled and determined experimentally – known quantity
5. Only other symbols used in two equations are p_o and n_o .
6. Two equations and two unknowns from which n and p need to be deduced.

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Carrier concentration calculations

Starting from the np product relation,

$$p = n_i^2 / n$$

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

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

Solving the quadratic equation for n then yields,

$$n = \frac{N_D - N_A}{2} + \left[\left(\frac{N_D - N_A}{2} \right)^2 + n_i^2 \right]^{1/2} \quad (2.29)$$

and

$$p = \frac{n_i^2}{n} = \frac{N_A - N_D}{2} + \left[\left(\frac{N_A - N_D}{2} \right)^2 + n_i^2 \right]^{1/2} \quad (2.30)$$

Only plus roots are retained, physically the carrier concentration must be greater than zero or equal to zero.

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Carrier concentration calculations

Above equations are general case solutions.

In many situations, it is possible to simplify these equations (2.29 and 2.30).

Special cases of specific interest:

1. Intrinsic semiconductor ($N_A = 0$, $N_D = 0$), equations simplify to $n_o = n_i$ and $p_o = n_i$

$n_o = p_o = n_i$ is the expected result, for equilibrium carrier concentration in an intrinsic semiconductor.

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Carrier concentration calculations

2. Doped semiconductor where either $(N_D - N_A) \sim N_D \gg n_i$
or $(N_A - N_D) \sim N_A \gg n_i$

Special case of general practical interest.

Unintentional doping levels in Si are such that the controlled addition of dopants routinely yields $N_D \gg N_A$ or $N_A \gg N_D$

Intrinsic carrier concentration in Si at room temperature is about $10^{10}/\text{cm}^3$, while the dominant doping concentration is seldom less than $10^{14}/\text{cm}^3$.

Thus the special case considered here is the usual case encountered in practice.

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Carrier concentration calculations

If $N_D - N_A \sim N_D \gg n_i$ square root term in eqn. (22 and 23) reduces to $N_D/2$ and,

$$n_o \sim N_D \quad (N_D \gg N_A, N_D \gg n_i)$$

$$p = n_i^2 / N_D \quad (2.31)$$

Similarly

$$p_o \sim N_A \quad (N_A \gg N_D, N_A \gg n_i)$$

$$n = n_i^2 / N_A \quad (2.32)$$

Numeric example, Si maintained at room temperature, uniformly doped with $N_D = 10^{15}/\text{cm}^3$ donors. Using above eqns. we can conclude, $n \sim 10^{15}/\text{cm}^3$ and $p \sim 10^5/\text{cm}^3$.

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Carrier concentration calculations

(3) Doped semiconductor where $n_i \gg |N_D - N_A|$

Systematic increase in ambient temperature causes a monotonic rise in intrinsic carrier concentration

At sufficiently high temperature, n_i will eventually equal and then exceed net doping concentration.

If $n_i \gg |N_D - N_A|$, square root in Eqns. 2.29 & 2.30 reduce to n_i and $n_o \sim p_o \sim n_i$

In other words all semiconductors becomes intrinsic at sufficiently high temperatures where $n_i \gg |N_D - N_A|$

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Determination of E_F (doped semiconductor)

Doped semiconductors (non-degenerate, dopants totally ionized)

General position of the Fermi levels in donor- and acceptor-doped semiconductors assumed to be

- (a) non-degenerate
- (b) in equilibrium
- (c) maintained at temperatures where the dopants are fully ionized.

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

Solving for $E_F - E_i$,

$$E_F - E_i = kT \ln(n_o/n_i) = -kT \ln(p_o/n_i) \quad (2.33) \quad 88$$

Determination of E_F (doped semiconductor)

Depending on the simplifications inherent of a particular problem, with appropriate carrier concentration solution, above eqn is used to determine the position of E_F

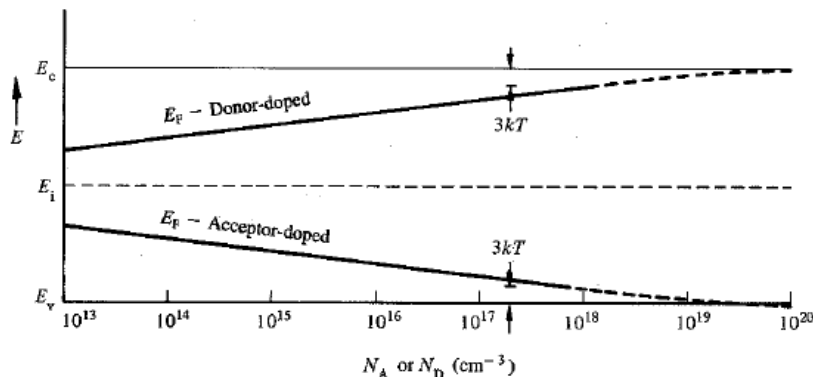
For example, $n_o \sim N_D$ in typical donor doped semiconductor and $p_o \sim N_A$ in typical acceptor doped semiconductor maintained at or near room temperature is used in above eqn.

$E_F - E_i = kT \ln(N_D/n_i)$	$\dots N_D \gg N_A, \quad N_D \gg n_i$	(2.34)
$E_i - E_F = kT \ln(N_A/n_i)$	$\dots N_A \gg N_D, \quad N_A \gg n_i$	

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Determination of E_F (doped semiconductor)



Fermi level systematically moves upward in energy from E_i with increasing donor doping, and systematically downward in energy from E_i with increasing acceptor doping

Fig. above refers to exact positioning of E_F in Si at room temperature as a function of doping concentration ($kT = 0.0259$ eV and $n_i = 10^{10}/\text{cm}^3$).

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