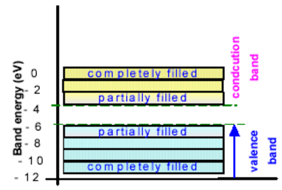
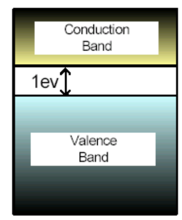
Lecture 3: Energy Band and Semiconductor Materials

- Energy band diagram is made of the highest energy bands of interest in considering electrical properties. The uppermost energy band is the ***conduction band*** (electrons moving freely once they are there). The middle band is the ***forbidden band*** in which no electrons occupy the band. The third band is the ***valence band*** that has the electron ready to be mobilized but yet need the energy to move.



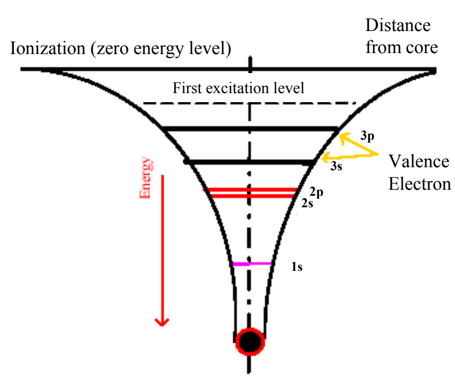
Semiconductor energy and partition



Silicone energy band

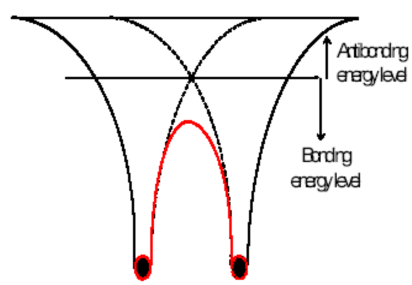
Si Energy Band

- Orbital energy model of one silicone atom along the energy levels of the various electrons can be presented in columbic potential well of the nucleus.
- When two atoms are completely isolated from each other, there is no interaction of electron wave function between them.



- When atoms bond together to form molecules of matter. The energy levels, which exist for single isolated atoms, split up to form *bands* of energy levels. Within each band there are still discrete permissible energy levels rather than a continuous band.

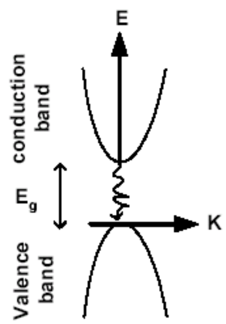
Columbic potential Well for one Si atom



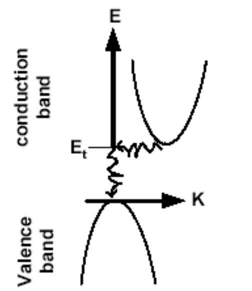
Direct and Indirect Semiconductors

- There are two classes of semiconductor energy bands; direct and indirect.
- In an indirect semiconductor such as GaAs, an electron in the conduction band can fall to an empty state in the valence band, giving off the energy Eg as a photon of light.
- An electron in the conduction band minimum cannot fall directly to the valence band maximum but must undergo a momentum change as well as changing its energy. For example, it may go through some defect state Et within the band gap.

Direct and Indirect Semiconductor



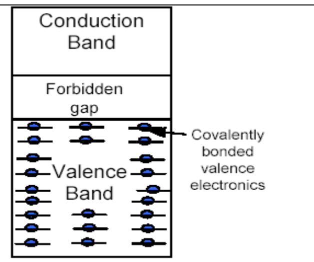
Direct electron transition in semiconductor



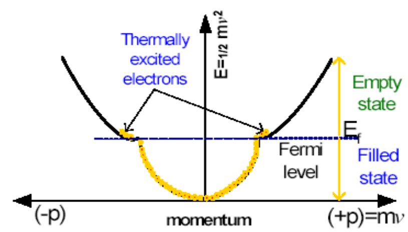
Indirect electron transition in semiconductor

Intrinsic Semiconductors

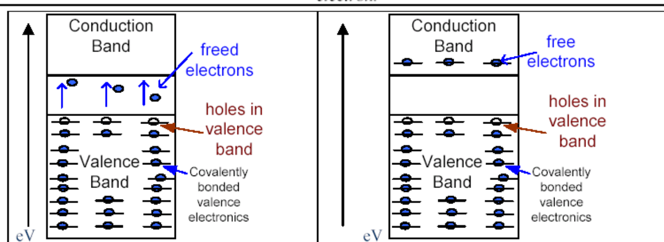
- For pure covalent bounded atoms, all of the valence electrons are tightly bound to the parent atoms and other atoms by covalent bonds. These electrons are not free to move through the crystal and, therefore, cannot conduct an electrical current. This is the case for intrinsic material at the absolute zero temperature (-273^{o}C or – 460^{o}F), which behaves as insulator.



Energy band of an intrinsic semiconductor at absolute temperature



Simplified energy- momentum curve for conduction electron in semiconductors at T=0°K .
Each point represents an occupied state. The Pauli exclusion principle limits occupation of each distinct state to one electron.



Generation of electron-hole pairs in an intrinsic semiconductor at room temperature

Carrier Concentration

- **Fermi-Dirac distribution function**
  - The distribution or probability density functions describe the probability with which one can expect particles to occupy the available energy levels in a given system. Of particular interest is the probability density function of electrons, called the *Fermi function*.

Fermi Function

- The Fermi-Dirac distribution function provides the probability of occupancy of energy levels by Fermions. Fermions are half-integer spin particles, which obey the Pauli exclusion principle. The Pauli exclusion principle postulates that only one Fermion can occupy a single quantum state.
- Fermi function provides the probability that energy level at energy, *E*, in thermal equilibrium with a large system, is occupied by an electron. Its temperature, T, and its Fermi energy, E_F, characterize the system.

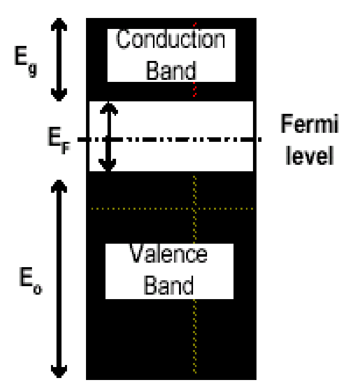
$$f(E) = \frac{1}{1 + e^{(E - E_F)/kT}}$$

Where
k is Boltzmann's constant ($k = 8.62 \times 10^{-5}$ eV/K or 1.38×10^{-23} J/K) and E_F is called the Fermi level.

Fermi level in an intrinsic semiconductor

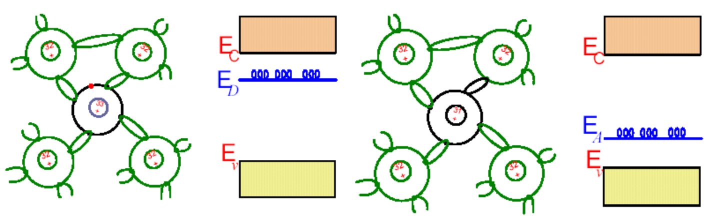
- Fermi energy level E_F lies in the middle of the energy gap i.e. midway between the conduction and valence band. With the following assumptions to evaluate E_F;

1. Width of energy bands is small as compared to forbidden energy gap.
2. Since bands widths are small, all levels in a band have the same energy.
3. Energies of all levels in valence band are zero
4. Energies of all levels in the conduction band are equal to Eg



Extrinsic Semiconductors

- Most of the used semiconductor material in the electronic devices has some impurities added to give it a predominance of either free electrons or holes. The process of adding impurities called ***doping***. Doping is performed after the semiconductor material been refined to a high degree of impurities.



N-type impurities *P-type impurities*

- Impurities alter the energy level within the band gap. For example, an impurity can introduce an energy level E_D (impurity level) very near the conduction band. This level is filled with electron at 0^oK, and very little thermal energy is required to excite these electrons to the conduction band. Thus at higher temperature, the electrons in the impurity level are donated to the conduction band. Impurity can provide large amount of electrons, thus semiconductors doped with a significant number of donor atoms will have $n_o >> (n_i,p)$ at room

Electron and Hole Concentrations at Equilibrium

- At equilibrium conditions, the concentration of electrons (number of electrons per unit volume) in the conduction band is the product of the density of states N(E) and the probability of occupancy *f*(E) and mathematically is given by

$$n_o = \int_{E_c}^{\infty} f(E)N(E)dE$$

where, *f*(E)N(E) is the density of states (cm^{-3}) in the energy range *dE*. The subscript O used to denote equilibrium conditions.

- For intrinsic material very few electrons occupy energy states far above the conduction band edge Ec. the probability of finding (hole) in the valence band {1-*f*(E)] decreases rapidly below Ev. Using the effective density of states *N*c to represent the all distributed electrons states in the conduction band, the concentration of electrons can be expressed as

$$n_o = N_c f(E_c)$$

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

So, the concentration is $n_o \cong N_c e^{-(E_o-E_F)/kT}$

where $$N_c = 2\left(\frac{2\pi m^*_n kT}{h^2}\right)^{3/2}$$

here m^*_n is the density-of –state effective mass for electrons.

Note that the electron concentration increases as E_F moves closer to the conduction

- By similar arrangements, the concentration of holes in the valence band is

$$p_o = N_v[1 - f(E_v)] \qquad p_o = N_v e^{-(E_F - E_V)/kT}$$

and

$$N_v = 2\left(\frac{2\pi m^*_p kT}{h^2}\right)^{3/2}$$

- The electron and hole concentration predicted above are valid whether the material is intrinsic or doped, provided thermal equilibrium is maintained. Thus for intrinsic material, E_F lies at the some intrinsic level E_i near the middle of the band gap and the intrinsic electron and hole concentrations are

$$n_i = N_c e^{-(E_c - E_i)/kT} \qquad p_i = N_v e^{-(E_i - E_V)/kT}$$

- The product of electron and holes concentration at equilibrium is constant for a particular material and temperature, even if the doping is varied:

$$n_o p_o = N_c N_v e^{-E_g/kT} = n_i p_i$$

- This yield that the intrinsic concentration is

$$n_i = \sqrt{N_c N_v} e^{-E_g/kT}$$

so practically $n_o p_o = n_i^2$

- In a general format,

$$n_o = n_i e^{-(E_F - Ei)/kT} \qquad p_o = n_i e^{-(E_i - E_F)/kT}$$

- This form of the above equations indicates that the electron concentration is n_i when E_F is at the intrinsic level E_i and that n_o increases exotically as the Fermi level moves away from Ei towards the conduction band. Similarly, the hole concentration p_o varies from n_i to larger values as E_F moves from E_i towards the valence band.

Majority and Minority Carriers

- An intrinsic of pure Germanium can be converted into P-type semiconductor by the addition of an acceptor impurity, which adds a large number of holes to it. A p-type material contains following charges:
  - Large number of positive holes – most of them is being added impurity with holes only a very small number of thermally generated ones.
  - A very small number of thermally generated electrons (the companions of the thermally generated holes).

- For this case, *holes* constitute majority carriers and electrons form minority carriers. Similarly in an N-type material, the number of electrons (both added and thermally generated) is much larger than the number of thermally generated holes. For this case, electrons constitute majority carriers and *holes* form minority carriers.

Conductivity of Intrinsic Semiconductor

- In semiconductor, current flow is due to the movement of electrons and holes in opposite directions.
- Even though the number of electrons equals the number of holes, hole mobility μh is practically half of electron mobility μe.
- In an intrinsic semiconductor of length L meter exposed to a electric field E (battery volt/length of conducting material) volt, the total current flow which is due to the sum of electron flow and hole flow, is given by

$$\boldsymbol{I = I_e + I_h}$$

Let v_e = drift velocity of electrons (m/s)
v_h = drift velocity of holes (m/s)
n_i = density of free electrons in an intrinsic semiconductor per m^3
p_i= density of holes in an intrinsic semiconductor per m^3
q = electron charge on coulomb
A = cross-section of the semiconductor in m^2

Also μe = *v*e/E and μh = vh/E and as *n*i = *p*i for pure semiconductor, then

$$I = n_i q(v_e + v_h)A = n_i q(\mu_e + \mu_h)AE$$
$$I = n_i q(\mu_e + \mu_h)AV / L$$

So the resistance is, $$\frac{V}{I} = \frac{L}{A}\frac{1}{n_i q(\mu_e + \mu_h)} = \rho\,\frac{L}{A}$$

where, ρ is the resistively of the semiconductor in ohm-m
The electrical conductivity of the semiconductor is the reciprocal of resistivity and is given by

$$\sigma_i = n_i q(\mu_e + \mu_h)$$

The current density *J* is given by *J* = *I*/*A so*

$$J = n_i q(\mu_e + \mu_h)E = \sigma_i E$$

From which the conductivity depends on two factors:
i- Number of current carriers present per unit volume, and
ii- The mobility of the current carriers

Conductivity of Extrinsic Semiconductor

- N-type semiconductors, the current density is

$$J_n = q(n_n \mu_e + p_n \mu_h)E$$

where, n_n and p_n represent the electron and hole densities in the N-type semiconductors after doping. The conductivity is given by

$$\sigma_n = J / E = q(n_n \mu_e + p_n \mu_h)$$

- As the electrons are a majority carrier, the conductivity could be approximated

$$\sigma_n = q n_n \mu_e$$

- P-type semiconductors, the current density is

$$J_p = q(n_p \mu_e + p_p \mu_h)E$$

where, n_p and p_p represent the electron and hole densities in the N-type semiconductors after doping. The conductivity is given by

$$\sigma_p = q(n_p \mu_e + p_p \mu_h)$$

- As the holes are a majority carrier, the conductivity could be approximated

$$\sigma_p = q n_p \mu_h$$

Charge Carriers

- Directed motion of charge carriers in semiconductors occurs through two mechanisms:
  (i) Charge drift under the influence of applied electric field
  (ii) Diffusion of charge from a region of high charge density to one of low charge density.
- When no electric field is applied to the semiconductor, the conduction of electrons (and holes) moves within the crystal with random motion and repeatedly collides with each other and the fixed ions. Due to randomness of the their motion, the net average velocity of these charge carriers is zero. Hence, no current exists in the crystal under this condition of no field.

Drift Carriers

- Once the electric field is applied, the charge carriers attain a directed motion that superimposed on their random thermal motion. This result in a net average velocity called ***drift velocity*** in the direction of the applied field (each to its attraction polarity).
- The drift velocity is proportional to electric field strength E, the constant of proportionality being called mobility μ. The exact relation of the two is $\upsilon = \mu E$.
- The total drift current will now be made of two components
  (i) A current density due to electron drift $J_e = q\mu_e nE$
  (ii) A current component due to hole drift $J_h = q\mu_h pE$
- The total current density due to electron and hole drift is

$$\mathbf{J} = \boldsymbol{J_e} + \boldsymbol{J_h} = \mathbf{qE}\,(\boldsymbol{n}\mu_e + \boldsymbol{p}\mu_h)$$

Diffusion of Carriers

- It is a force-free process based on non-uniform distribution of charge carriers in a semiconductor crystal. It is gradual floe of charge from a region of high density to a region of low density. This flow of ***diffusion of carriers*** is proportional to the carrier density gradient, the constant of proportionality being called diffusion constant or diffusion coefficient D that has a unit of m^2/s.
- The total diffusion current density is made of two components

  (iii) A current density due to electron diffusion $J_e = qD_e \, dn/dx$

  (iv) A current density due to holes diffusion $J_h = qD_h \, dp/dx$

Combined Drift and Diffusion of Currents

$$J_e = q\mu_e nE + qD_e \, dn/dx \qquad J_h = q\mu_h pE - qD_h \, dp/dx$$

- Relation between D and μ

  Both diffusion constant and mobility are statically thermodynamic phenomena and are related to each other

$$\mu_e = \frac{q}{kT} D_e \quad \text{and} \quad \mu_h = \frac{q}{kT} D_h$$

or

$$\frac{D_e}{\mu_e} = \frac{D_h}{\mu_h} = \frac{kT}{q} = \frac{T}{11600}$$

This relation is known as **Einstein's equation**.

Properties of Si, Ge and GaAs at T=300K

Property	Unit	Si	Ge	GaAs
Density of Atoms	cm^{-3}	5×10^{22}	4.4×10^{22}	2.2×10^{22}
Energy Gap	eV	1.12	0.66	1.42
Effective mass				
electron		1.182	0.553	0.0655
hole		0.81	0.357	0.524
Effective Density State	cm^{-3}			
conduction band		3.22×10^{19}	1.03×10^{19}	4.21×10^{17}
valence band		1.83×10^{19}	5.35×10^{18}	9.52×10^{18}
Intrinsic Carrier Density	cm^{-3}	1×10^{10}	2.17×10^{13}	2.49×10^{6}
Mobility at low doping	$cm^{-3}/(V\text{-}s)$			
electron		1350	3900	8800
hole		480	1900	400
Breakdown Field	V/cm	3×10^{5}	10^{5}	4×10^{5}
Relative Permittivity		11.8	15.8	13.1
Melting Point	^{o}C	1410	940	1240

Physical Constants and Factors

Quantity	Symbol	Value
Boltzmann Constant	k	1.38066×10^{-23} J/K
Boltzmann Constant	k/q	8.61738×10^{-5} eV/K
Magnitude of Electronic Charge	q	1.602×10^{-19} C
Electronvolt	eV	1.602×10^{-19} J
Permittivity of Vacuum	ε_o	8.854×10^{-12} F/m
Planck's Constant	h	6.626×10^{-34} J-s
Thermal Voltage	Vt = kT/q	0.02586 (*T=300K*)

Band Gap Variation with Temperature

$$E_g(T) = E_g(0) - \frac{T^2\alpha}{(T+\beta)}(eV)$$

Material	$E_g(0)$	$\alpha(10^{-4})$	β
GaAs	1.519	5.405	204
Si	1.17	4.73	636
Ge	0.7437	4.774	235

Fermi Level

- Intrinsic

$$E_i = E_F = \frac{E_C + E_V}{2} + kT\ln(N_V / N_C)$$

- Extrinsic

N-type $\quad E_F - E_i = kT\ln(N_D / n_i)$

P-type $\quad E_i - E_F = kT\ln(N_A / n_i)$