# Chapter I – Some fundamentals of semiconductors and optics

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# **Part I – Semiconductors**

## Why Semiconductors ?

- Semiconductors are the materials between metal and insulator.
- The conductivity can be flexibly adjusted by doping impurities.
- Different impurity gives different conductivity behaviors, such as hole and electron.
- Structure is almost perfect so that the materials are capable to be manipulated.
- The built-in field inside a semiconductor is controllable from outside.
- It's compact (small size) and has the capability for integration.
  - high-speed ICs, nano-technology applications, and quantum devices.
- Technology template (can be made by standard processing)
  - processing, packaging, and testing are ready and very suitable for mass production.

 $\begin{array}{ll} \mbox{Resistivity, $\rho$} \left(\Omega\ cm\right) & \rho_{Insulator} > 10^4\ \Omega\ cm\ \rho_{Semiconductor} > 10^{-2}\ \mbox{--}\ 10^4\ \Omega\ cm \\ \\ & \rho_{metal} < 10^{-6}\ \Omega\ cm \end{array}$ 

## **Periodic table of atoms**





SiC, GaAs, BN, InAs, GaP, CdS, CdSe, ZnS, ZnSe, PbS, and PbTe

## **Crystal Structure**

#### **Cubic class of crystal**



- The semiconductor materials we will study are single crystal, that is, the atoms are arranged in a 3-D periodic fashion. The periodic arrangement of atoms in a crystal is called a lattice.
- For a given semiconductor, there is a unit cell that is representative of the entire lattice; by repeating the unit cell throughout the crystal, one can generate the entire lattice.

#### **Miller index**

Directions in crystals of the cubic class are very conveniently described in terms of Miller notation. For example, any plane in space can be represent by:

 $\frac{x}{a} + \frac{y}{b} + \frac{z}{c} = 1$  where *a*, *b*, and *c* are the intercepts made by the plane at *x*, *y*, and *z* axes.

Writing *h*, *k* and *l* as the reciprocals of these intercepts, the plane can be described by

$$hx + ky + lz = 1$$

The Miller indices for this plane are written as (*hkl*).



#### **Atom arrangements of semiconductors**





The ultimate tensile strength of Si  $(0.35 \times 10^{10} \text{ dyn/cm}^2)$  is maximum in <111> directions. In addition, the modulus of elasticity in the <111> directions is higher than that in the <110> or <100> directions  $(1.9 \times 10^{12} \text{ dyn/cm}^2, 1.7 \times 10^{12} \text{ dyn/cm}^2, \text{ and } 1.3 \times 10^{12} \text{ dyn/cm}^2,$  respectively). As a result, Si tends to cleave on the {111} planes.

### **Energy Band of Semiconductors**



**Two close-up atoms** 

The energy level of an isolated hydrogen atom are given by Bohr model:

$$E_{H} = \frac{-m_{0}q^{4}}{8\varepsilon_{0}^{2}h^{2}n^{2}} = \frac{-13.6}{n^{2}}eV$$

where *n* is a positive integer called the principle quantum number. The discrete energies are -13.6 eV for the ground level (n = 1), -3.4 eV for the first excited level (n = 2), etc.

The identical energy level of two closed-up atoms will split into two levels by the interaction between atoms. When we bring N atoms to form a crystal, the *n*-fold degenerate energy level will split into N separate but closely spaced levels due to atom interaction. This results in an essentially continuous band of energy.

#### **Example:** Alkali metals and insulators



But with 2N energy levels

For insulators, valence electrons completely fill an allowed energy band.





If  $E_g$  is too large, no electrons can gain enough energy to translate from the lower energy band to the higher energy band.

**Low conductivity** 

#### k-space diagram

For a free electron, the kinetic energy *E* is given by

$$E = \frac{p^2}{2m_0}$$
 where *p* is the particle momentum and  $m_0$  is the free electron mass.

However, the effective mass of a conduction band electron is different from the mass of a free electron. The energy-momentum relationship of a conduction electron can be written as

 $E = \frac{\overline{p}^2}{2m_n}$  where  $\overline{p}$  is the crystal momentum and  $m_n$  is the free electron mass.



*E-p* (or k) plot of a free particle



Electrons traveling in different directions encounter different potential patterns and therefore different *k*-space boundaries.

#### **Energy band diagram**



- For direct band material, transitions between two allowed bands can take place with no change in crystal momentum *p*.
- A transition in an indirect bandgap material must necessarily include an interaction with the crystal so that crystal momentum is conserved.

• With a known *E-p* relationship, one can obtain the effective mass from the second derivative of *E* with respect to *p* 

$$m_n = \left[\frac{d^2 E}{d\overline{p}^2}\right]^{-1}$$
 The narrower the parabola, the smaller the effective mass.

#### **Density of state of bulk semiconductors**



$$L/\lambda_{x} = m \qquad L/\lambda_{y} = n \qquad L/\lambda_{z} = k \qquad \lambda_{i} : \text{ wavelength of electron, } i = x, y,$$

$$Use \ \lambda_{i} = h/p_{i} \implies Lxp_{x} = hxm \text{ or } Lxdp_{x} = h$$

$$Lxp_{y} = hxm \text{ or } Lxdp_{y} = h \implies L^{3}xdp_{x}xdp_{y}xdp_{z} = h^{3}$$

$$Lxp_{z} = hxk \text{ or } Lxdp_{z} = h$$

Ζ.

The volume of an allowed state in momentum space is  $h^3$ :

$$\therefore \quad N(E)dE = 2 \times \frac{4\pi p^2 dp}{h^3} = 4\pi (\frac{2m_n}{h^2})^{3/2} \sqrt{E} dE \implies \quad N(E) = 4\pi (\frac{2m_n}{h^2})^{3/2} \sqrt{E}$$

## **Doping on Semiconductors**



**Pure Si-crystal** 

**Doped Si-crystal** 

### **Activation of doping**



Valence band

Due to the thermal agitating, the carrier concentration and the type of carrier can be controlled by impurity doping!!!

#### **Ionization energies of impurities in Si**

![](_page_14_Figure_1.jpeg)

**Exercise of hydrogen atom are**  $E = -\frac{mq^4}{8a^2h^2\varepsilon_o^2}$ 

$$E_{ionization} = \frac{13.6}{\varepsilon_r^2} \frac{m_n}{m_o}$$
  
for Si,  $m_n = 0.06 m_o$  and  $\varepsilon_r = 11.8$ ,  $\Box$   $E_{ionization} \sim 0.06 \text{ eV}$ 

#### **Ionization energies for group III and V impurities**

| Dopant         | Р     | As    | Sb    | В     | Al    | Ga    | In   |
|----------------|-------|-------|-------|-------|-------|-------|------|
| Acceptor level |       |       |       | 0.045 | 0.057 | 0.065 | 0.16 |
| Donor level    | 0.044 | 0.049 | 0.039 |       |       |       |      |

#### **Fermi-Dirac distribution**

Thermal equilibrium: the total energy of a semiconductor is a function only of crystal temperature.

**Fermi-Dirac distribution :** 
$$f(E) = \frac{1}{1 + \exp(\frac{E - E_F}{kT})}$$
  $E_F$ : Fermi energy

The probability of a state with energy *E* occupied by an electron at temperature T. The Fermi function only represents a probability of occupancy. It does not contain any information about the states available for occupancy and, therefore, can not by itself specify the electron population at a given energy.

![](_page_15_Figure_4.jpeg)

- $E_F$ : the highest filled state at T= 0°K (from the Pauli's exclusion principle)
- When  $E = E_{I\!\!P} f(E) = 0.5$ .
- Only the electrons near the Fermi's level have the contribution to current conduction.

• 
$$n = \int_0^{Etop} n(E) dE = \int_0^{Etop} N(E) f(E) dE$$

## **Effective Density of States**

#### The electron carrier density

$$n = \int N(E) \cdot f(E) \cdot dE \quad \text{where} \quad N(E) = 4\pi \left(\frac{2m_{e,k}}{h^2}\right)^{3/2} \times \sqrt{E} \quad \text{and} \quad f(E) = \frac{1}{1 + \exp\left(\frac{E - E_F}{kT}\right)}$$
Density of states Fermi-Dirac distribution
If  $E_{d,v} > 3kT$ ,  $\rightarrow f(E) \approx e^{-(E - E_F)/kT}$  or If  $E_{d,v} < 3kT$ ,  $\rightarrow f(E) \approx 1 - e^{-(E_F - E)/kT}$ 

$$\Rightarrow \quad n = \int N(E) \cdot f(E) \cdot dE \approx 4\pi \left[\frac{2m_e}{h^2}\right]^{3/2} \int_{E_C}^{\infty} \sqrt{E} \exp\left(-\frac{E - E_F}{kT}\right) dE$$

$$= 2 \left[\frac{2\pi m_e kT}{h^2}\right]^{3/2} e^{-(E_F - E_F)/kT}$$

$$p = 2 \left[\frac{2\pi m_e kT}{h^2}\right]^{3/2} e^{-(E_F - E_F)/kT}$$

$$p \approx N_C \times e^{-\frac{E_F - E_F}{kT}}$$
where  $N_{C,V} = 2 \times \left(\frac{2\pi m_{e,k}kT}{h^2}\right)^{3/2}$ 
Effective density of state

If  $E_{d,v} > 3kT$ ,  $\rightarrow f(E) \approx e^{-(E-E_F)/kT}$ 

In n-type material that is not too highly doped, few of the allowed states in the conduction band are filled. The Fermi function in the conduction band is very small, and the Fermi level is well below the bottom of the conduction band. Then  $(E_c - E_f) >> kT$ , and the Fermi function reduces to the mathematically simpler Maxwell-Boltzmann distribution function. That is

 $f(E) \approx e^{-(E-E_F)/kT}$ 

At energies well above the Fermi level the fraction of available states that are occupied is so small that the exclusive-principle limitation has no practical effect and Maxwell-Boltzmann statistics are applicable.

### **Free carriers of semiconductors**

![](_page_18_Figure_1.jpeg)

![](_page_19_Figure_0.jpeg)

![](_page_19_Figure_1.jpeg)

![](_page_19_Figure_2.jpeg)

States at energy *E* which are less than  $E_F$  are mostly filled; States at energy *E* which are larger than  $E_F$  are mostly unoccupied.

## **Example: Mass action law**

$$n \approx N_C \times e^{-\frac{E_C - E_F}{kT}}$$

$$p \approx N_V \times e^{-\frac{E_F - E_V}{kT}}$$

$$n \cdot p = n_i^2 = N_c \cdot N_v \cdot \exp(-\frac{E_g}{kT})$$

At room temperature,

$$kT \sim 25 \text{ meV} \implies exp(-3kT/kT) \sim 0.05$$
  
 $n_i (\text{GaAs}) = 1.2 \times 10^6 \text{ cm}^{-3} < n_i (\text{Si}) = 1.45 \times 10^{10} \text{ cm}^{-3}$ 

- n, p are quite sensitive to the  $E_g$ , temperature and impurity level !!!
- The electrical properties can be controlled by impurity over a few orders of magnitude !!!

**Example: Intrinsic level** 

$$n = p \equiv n_i \rightarrow N_C \times e^{-\frac{E_C - E_F}{kT}} = N_V \times e^{-\frac{E_F - E_V}{kT}} \rightarrow E_F = \frac{E_C + E_V}{2} + \frac{kT}{2} \times \ln\left[\frac{N_V}{N_C}\right]$$
$$= \frac{E_C + E_V}{2} + \frac{3kT}{4} \times \ln\left[\frac{m_p}{m_e}\right]$$

At RT, the second term is much smaller than the  $E_g$ . Hence, the intrinsic Fermi level  $E_i$  lies very close to the middle of bandgap.

For n-type semiconductor

$$n_{i} = N_{C} \times e^{-\frac{E_{C}-E_{i}}{kT}}$$
 or 
$$N_{D} = n_{i} \times e^{\frac{E_{Fn}-E_{i}}{kT}}$$
  $E_{i}$ : intrinsic level   
 
$$N_{D} = N_{C} \times e^{-\frac{E_{C}-E_{Fn}}{kT}}$$
 or 
$$E_{Fn}-E_{i} / N_{D} /$$
 For p-type semiconductor

$$\Rightarrow \begin{array}{c} p_i = N_V \times e^{-\frac{E_i - E_V}{kT}} \\ N_A = N_V \times e^{-\frac{E_{F_p} - E_V}{kT}} \end{array} \quad \text{or} \qquad N_A = p_i \times e^{\frac{E_i - E_{F_p}}{kT}} \quad \Rightarrow E_i - E_{F_p} \uparrow \quad N_A \end{array}$$

**Problem:** A Si ingot is doped with 10<sup>16</sup> As atoms/cm<sup>3</sup>. Find the carrier concentration and Fermi level at 300K.

At 300 K, we can assume complete ionization of impurity atoms. We have  $n \sim N_D = 10^{16} \text{ cm}^{-3}$ 

Use 
$$p = \frac{n_i^2}{N_D} = 2.1 \times 10^4 cm^{-3}$$
  
 $E_C - E_F = kT \times \ln\left[\frac{N_C}{N_D}\right] = 0.206 eV > 3kT$   
 $E_F - E_i = kT \times \ln\left[\frac{N_D}{n_i}\right] = 0.354 eV$ 

If both donor and acceptor impurities present simultaneously, the impurity that is present in a greater concentration determines the type of conductivity in the semiconductor.

## **Example: Charge neutrality**

If charge neutrality in a region where all dopant are ionized,

$$\begin{split} N_{D} + p &= N_{A} + n \quad or \quad n - p = N_{D} - N_{A} \\ From & mass - action - law \to p = \frac{n_{i}^{2}}{n} \\ \to n - \frac{n_{i}^{2}}{n} &= N_{D} - N_{A} \quad or \\ n &= \frac{N_{D} - N_{A}}{2} + \sqrt{\left(\frac{N_{D} - N_{A}}{2}\right)^{2} + n_{i}^{2}} \quad \text{and} \quad p = \frac{N_{A} - N_{D}}{2} + \sqrt{\left(\frac{N_{A} - N_{D}}{2}\right)^{2} + n_{i}^{2}} \end{split}$$

In general, the net impurity concentration  $|N_D - N_A|$  is larger than the intrinsic carrier concentration. Therefore the above equations can be simplified to

$$n \approx N_D - N_A$$
 or  $p \approx N_A - N_D$ 

## **Problem: Compensation**

A silicon crystal is known to contain 10<sup>-4</sup> atomic percentage of arsenic (As) as an impurity. It then receives a uniformity doping of 3 ×10<sup>16</sup> cm<sup>-3</sup> phosphorus (P) atoms and subsequent uniformity doping of 10<sup>18</sup> cm<sup>-3</sup> boron (B) atoms. All dopant are activated by thermal annealing.

Si has 5 ×10<sup>22</sup> atoms cm<sup>-3</sup>, 10<sup>-4</sup> atomic percentage

Si is doped to a concentration of  $5 \times 10^{22} \times 10^{-6} = 5 \times 10^{16}$  As atoms cm<sup>-3</sup>

The added doping of 3×10<sup>16</sup> P atoms cm<sup>-3</sup>,

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\Rightarrow 5 \times 10^{16} + 3 \times 10^{16} = 8 \times 10^{16} \text{ n-type atoms cm}^{-3}
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p-type doping is 10<sup>18</sup> cm<sup>-3</sup>,

 $\Rightarrow$  p = 10<sup>18</sup> - 8×10<sup>16</sup> = 9.2×10<sup>17</sup> cm<sup>-3</sup>

# **Carrier transport phenomena**

## **Carrier Drift**

#### Mobility

Under thermal equilibrium, the average thermal energy of a conduction electron can be given by:

$$\frac{1}{2}m_e v_{th}^2 = \frac{3}{2}kT \quad \text{where } v_{th} \text{ is the average thermal velocity.}$$

At 300 K, the thermal velocity is about  $10^7$  cm/s for Si and GaAs. Electrons in semiconductor are therefore moving rapidly in all direction. The thermal motion of an electron can be visualized as a succession of random scattering from collisions with lattices, impurities, and other scattering centers. The average distance between collisions is called mean free path, and the average time between collision is called mean free time,  $\tau_{cn}$ .

![](_page_26_Figure_5.jpeg)

Electrons exchange energy when collide with the lattice and drop toward their thermal equilibrium positions. The energy lost in each collision is much less than the mean thermal energy of the electrons.  $F \cdot \Delta t = m \cdot \Delta v$ 

$$-qE\tau_{cn} = m_n^* \cdot v_d \quad \text{or} \quad v_d = \frac{-qE\tau_{cn}}{m_n^*}$$
  
Let mobility  $\mu_n = -\frac{v_d}{E} = q \times \frac{\tau_{cn}}{m_n^*}$ 

where  $v_d$  is the drift velocity in an applied field.

Mobility is an important parameter for carrier transport because it describes how strongly the motion of an electron is influenced by an electric field.

#### **Example:** hot carriers

For Si semiconductor, electrons with  $\mu_n = 1400 \text{ cm}^2/\text{Vsec}$  have a drift velocity of only 1.5 % of the thermal velocity if E = 100 V/cm. Typical thermal velocity at RT is 10<sup>7</sup> cm/sec.

$$\mathbf{E} \not \quad \mathbf{v_d} \not \quad \mathbf{E_k} = \frac{1}{2} m_n^* v_d^2 \not \uparrow$$

When electrons attain energy above the ambient thermal energy, they are often characterized as hot carriers with an effective temperature  $T_e$ . When the energy of the hot carriers reaches a critical value, a new scattering process (optical phonon scattering) become important. This new scattering process can effectively transfer energy from the hot carriers to the lattice, and it is the major reason that the drift velocity approaches a limit value at high field conditions.

**Current density:** 

$$\vec{J}_n = \sum_i q \vec{v}_i = -nq \vec{v}_d = nq \mu_n \vec{E}$$
$$\vec{J}_p = pq \mu_p \vec{E}$$
$$\vec{J}_{tot} = \vec{J}_n + \vec{J}_p$$

## **Empirical expression of** *e***-***h* **mobility**

$$\mu_n = 88 \times T_n^{-0.57} + \frac{7.4 \times 10^8 T^{-2.33}}{1 + [N/(1.26 \times 10^{17} T_n^{2.4})] \times 0.88 \times T_n^{-0.146}}$$
$$\mu_p = 54.3 \times T_n^{-0.57} + \frac{7.4 \times 10^8 T^{-2.23}}{1 + [N/(2.35 \times 10^{17} T_n^{2.4})] \times 0.88 \times T_n^{-0.146}}$$

| N (cm <sup>-3</sup> ) | Arsenic | Phosphorus | Boron |
|-----------------------|---------|------------|-------|
| 1013                  | 1423    | 1424       | 486   |
| 1014                  | 1413    | 1416       | 485   |
| 1015                  | 1367    | 1374       | 478   |
| 1016                  | 1184    | 1194       | 444   |
| 1017                  | 731     | 727        | 328   |
| 1018                  | 285     | 279        | 157   |
| 1019                  | 108     | 115        | 72    |

#### Resistivity

![](_page_30_Figure_1.jpeg)

$$I = JA = qn\nu_{d}A = qn\mu_{n}EA = qn\mu_{n}\frac{V}{L}A = \sigma\frac{A}{L}V$$
$$J = J_{n} + J_{p} = (qn\mu_{n} + qp\mu_{p}) \cdot E$$

$$\rho = \frac{1}{\sigma} = \frac{1}{qn\mu_n + qp\mu_p} \qquad n, p \uparrow \mu_{n,p} \uparrow \Rightarrow \rho \downarrow$$

Carrier concentration and mobility are the two most important factors which affect the conductivity of a semiconductor.

$$R = \rho \frac{L}{A} = \rho \frac{L}{t \times w} \qquad \text{Let's choose } L = w \to \qquad R = \rho \frac{L}{A} = \rho \frac{1}{t \times w} = \rho \frac{1}{t} \equiv R_s \quad \Omega/\Box$$
Sheet resistance

#### **Four-point probe**

The four-point probe technique can also be used to measure resistance of a connection where contact resistance  $(R_c)$  of probes can not be ignored. As shown in the following figure, probe 1 and probe 2 are used to inject current to the contact pads, and probe 3 and probe 4 are used to measure the voltage difference between the two pads. Please show that the resistance  $(R_l)$  between the two pads can be readily obtained by dividing the voltage measured by probe 3 and 4 to the current injected by probe 1 and 2. The contact resistance of the probes are canceled by using the technique.

![](_page_31_Figure_2.jpeg)

## **Carrier Diffusion**

![](_page_32_Figure_1.jpeg)

Because of the finite temperature, the electrons have random motions. The gradient of carrier concentration will result in a net carrier flow. Diffusion current is generally not an important consideration in metals because of their high conductivity. The lower conductivity and the possibility of non-uniform density of carriers and of carrier energies, however, often makes diffusion a very important process affecting current flow in semiconductors.

![](_page_32_Figure_3.jpeg)

#### **Current density equations**

![](_page_33_Figure_1.jpeg)

The carrier-transport process involves not only the drift and also the diffusion processes !!!

#### **Total current is:**

$$J_{n} = nq\mu_{n}E + qD_{n}\frac{dn}{dx} \qquad J_{p} = pq\mu_{p}E - qD_{p}\frac{dp}{dx}$$
$$J_{cond} = J_{n} + J_{p}$$

## **Continuity Equations**

We are now ready to consider the over all effect when drift, diffusion, and recombination occur simultaneously in a semiconductor material.

![](_page_34_Figure_2.jpeg)

The number of hole in the slice may increase due to net current flow into the slice and net carrier generation in the slice. The over all rate of holes increase include three components: the change of hole flux at x, plus the rate at which holes are generated, minus the rate at which they are recombined with electrons in the slice.

$$\frac{\partial p_n}{\partial t} dx dy dz = -\frac{\partial F_{px}}{\partial x} dx dy dz + G_p dx dy dz - \frac{p_n - p_{n0}}{\tau_p} dx dy dz$$

![](_page_35_Figure_0.jpeg)

![](_page_35_Figure_1.jpeg)

![](_page_35_Figure_2.jpeg)

$$\frac{\partial n_p}{\partial t} = n_p \mu_n \frac{\partial E}{\partial x} + \mu_n E \frac{\partial n_p}{\partial x} + D_n \frac{\partial^2 n_p}{\partial x^2} + G_n - \frac{n_p - n_{po}}{\tau_n}$$
$$\frac{\partial p_n}{\partial t} = -p_n \mu_p \frac{\partial E}{\partial x} - \mu_p E \frac{\partial n_p}{\partial x} + D_p \frac{\partial^2 p_n}{\partial x^2} + G_p - \frac{p_n - p_{no}}{\tau_p}$$

#### In addition to the continuity equations, Poisson equation must also be satisfied.

$$\frac{\partial E}{\partial x} = \frac{\rho_s}{\varepsilon_s}$$
 and  $\rho_s = q \times (p - n + N_D^+ - N_A^-)$ 

where  $\rho_s$  is the space charge density and  $\varepsilon_s$  is the dielectric permittivity.

## **Steady-state injection from one side**

![](_page_37_Figure_1.jpeg)

At steady state,

$$\frac{\partial p_n}{\partial t} = 0 = D_p \frac{\partial^2 p_n}{\partial x^2} - \frac{p_n - p_{n0}}{\tau_p}$$

and the B.C. are:  $p_n(x = 0) = p_n(0)$  and  $p_n(\infty) = p_{n0}$ 

The solution of  $p_n(x)$  is  $p_n(x) = p_{n0} + [p_n(0) - p_{n0}]e^{-x/L_p}$  where  $L_p$  is called the diffusion length.

If the boundary conditions are changed so that all excess carriers at x = W are extracted, that is,  $p_n(W) = p_{n0}$ , then the solution becomes

![](_page_37_Figure_7.jpeg)

$$p_{n}(x) = p_{n0} + [p_{n}(0) - p_{n0}] \frac{\sinh[\frac{W - x}{L_{p}}]}{\sinh(W/L_{p})}$$
$$J_{p} = -qD_{p}\frac{\partial p_{n}}{\partial x}|_{W} = q[p_{n}(0) - p_{n0}]\frac{D_{p}}{L_{p}}\frac{1}{\sinh(W/L_{p})}$$

# **Metal-semiconductor Contacts**

## **Equilibrium in Electronic Systems**

At thermal equilibrium, Fermi level is constant throughout a system.

![](_page_39_Figure_2.jpeg)

he filled state density is  

$$n = g \bullet F_D \bullet_{\text{Fermi function}}$$
 The vacant state density is  
 $v = g \bullet (1 - F_D)$  Allowed electron state density

We now consider that the two systems are brought in intimate contact. Equilibrium is reached when there is no net transfer of electrons at any energy.

$$\therefore \quad n_1 v_2 = n_2 v_1 \quad or \quad F_{D1} g_1 (1 - F_{D2}) g_2 = F_{D2} g_2 (1 - F_{D1}) g_1$$
$$\implies \quad F_{D1} = F_{D2} \quad or \quad E_{F1} = E_{F2}$$

#### **Example:** inhomogeneously doped semiconductor

Consider now the energy band diagram at thermal equilibrium for an n-type semiconductor doped with  $N_{d1}$  for 0 < x < a and with  $N_{d2}$  for x > a. Please draw the energy band diagram of this system.

![](_page_40_Figure_2.jpeg)

![](_page_41_Figure_0.jpeg)

![](_page_41_Figure_1.jpeg)

In the metal, the Fermi level is immersed within a continuum of allowed states, while in semiconductor, the density of state is negligible at the Fermi level.

![](_page_41_Figure_3.jpeg)

- At thermal equilibrium, there is no net transfer of electrons at any energy. Therefore the Fermi level is constant throughout the system.
- If  $\phi_M$  is larger than  $\phi_S$ , e will flow from semiconductor to metal, and this will causes the  $E_c$  to bend upward.
- If  $\phi_S$  is larger than  $\phi_M$ , e will flow from metal to semiconductor, and this will causes the  $E_c$  to bend downward.

#### **Band diagram of metal-semiconductor interface**

![](_page_42_Figure_1.jpeg)

- $\phi_i$ : build-in protential =  $\phi_M \phi_s = \phi_M X (E_C E_{fn})$
- $\phi_B$  : barrier height =  $\phi_M X$
- $x_d$ : depletion region width
- Our development thus far has relied on the fact that basic band structure of the two materials are unchanged near the surface.

#### **Charge, Depletion, and Capacitance**

#### n-type semiconductor

![](_page_43_Figure_2.jpeg)

![](_page_43_Figure_3.jpeg)

**Consider the Poisson equation:** 

$$\frac{d^2\phi}{dx^2} = -\frac{q}{\varepsilon}(N_d^+ - N_a^- + p - n)$$

For  $x < x_d$ ,

$$n = N_c \times e^{-[E_C(x) - E_F]/kT}$$

**For x >> 0,** 

$$n(\infty) = N_d = N_c \times e^{-(E_C(\infty) - E_F)/kT}$$
  
or 
$$n = N_d \times e^{-[E_C(x) - E_C(\infty)]/kT} = N_d \times e^{-q\phi(x)/kT}$$
$$\frac{d^2\phi}{dx^2} = -\frac{q}{\varepsilon} N_d (1 - e^{-q\phi(x)/kT})$$

#### **Complete Depletion Approximation**

![](_page_44_Figure_1.jpeg)

If  $\phi_i$  is large enough to deplete the free carriers in the junction, the complete depletion approximation is then valid.

![](_page_45_Figure_0.jpeg)

$$\phi(x_d) = \phi_i = \frac{qN_d}{\varepsilon_s} \frac{x_d^2}{2} \quad or \quad x_d = \sqrt{\frac{2\phi_i\varepsilon_s}{qN_d}}$$
$$\implies N_d \uparrow \quad x_d \downarrow$$

$$E(x) = -\frac{d\phi(x)}{dx} = -\frac{qN_d}{\varepsilon_s} x_d (1 - \frac{x}{x_d})$$

$$E = -\frac{qN_d}{\varepsilon_s} x_d (1 - \frac{x}{x_d})$$

or 
$$E_{\max} = -\frac{qN_d}{\varepsilon_s} x_d$$

#### **Applied bias and capacitance**

When a bias is applied to a metal-n-type semiconductor junction, we need to consider the non-equilibrium condition of the junction. Under a bias condition, the barrier is reduced when the metal is biased positively with respect to the semiconductor, and it is increased under bias of the opposite polarity.

![](_page_46_Figure_2.jpeg)

Under the bias conditions, the voltage drop across the space-charge region is changed to  $(\phi_i - V_a)$ , then the space charge density in the semiconductor changes accordingly.

$$Q = qN_{d}x_{d} = \sqrt{2q\varepsilon_{s}N_{d}(\phi_{i} - V_{a})}$$

$$C = \frac{\partial Q}{\partial V_{a}} = \sqrt{\frac{q\varepsilon_{s}N_{d}}{2(\phi_{i} - V_{a})}} = \frac{\varepsilon_{s}}{x_{d}} \quad or \quad (\phi_{i} - V_{a}) = \frac{q\varepsilon_{s}N_{d}}{2C^{2}}$$

## **Example: Complete depletion approximation**

Complete depletion approximation is valid only when the build-in potential is large enough to deplete the free carriers in the space-charge region.

In equilibrium,

$$J_n = 0 = q\mu_n nE_x + qD_n \frac{dn}{dx} \to E_x = -\frac{D_n}{\mu_n} \frac{1}{n} \frac{dn}{dx} = -\frac{kT}{q} \frac{1}{n} \frac{dn}{dx}$$
  
Use  $E_x = -\frac{d\phi}{dx} \to d\phi = \frac{kT}{q} \frac{dn}{n} \to \Delta\phi = \frac{kT}{q} \ln \frac{n'}{n}$ 

For  $n' = 10^{18}$  cm<sup>-3</sup>,  $n = 10^{16}$  cm<sup>-3</sup>, and the variation of the dopant concentration is over the range of a few hundred nanometers,

$$\rightarrow \Delta \phi = 0.12V \rightarrow E_x = -\frac{\Delta \phi}{\Delta x} = 2400V/cm$$
$$\frac{d^2 \phi}{dx^2} \approx 5 \times 10^7 V/cm^2 = -\frac{q}{\varepsilon_s} (N_D - n) \rightarrow \left| N_D - n \right| \approx 10^{15} cm^{-3} \rightarrow N_D \approx n \gg 0$$

Under this condition, the complete depletion approximation is not valid.

## **I-V Characteristics**

### **Drift-diffusion approach**

$$J_{x} = q[n\mu_{n}E_{x} + D_{n}\frac{dn}{dx}] = qD_{n}\left[\frac{-qn}{kT}\frac{d\phi}{dx} + \frac{dn}{dx}\right]$$
$$\stackrel{\uparrow}{\underset{D_{n}}{=}} = \frac{kT}{q}$$
$$\times e^{-\frac{q\phi}{kT}}, \quad and \quad \int_{0}^{x_{d}} [\dots]dx \quad \Rightarrow J_{x}\int_{0}^{x_{d}} e^{-\frac{q\phi}{kT}}dx = qD_{n}[ne^{-\frac{q\phi}{kT}}]_{0}^{x_{d}}$$

**B.C.**:  $\phi(x_d) = \phi_i - V_a = \phi_B - \phi_n - V_a$ , and  $\phi(0) = 0$ ,

$$n(x_d) = N_d = N_C \cdot e^{-\frac{q\phi_n}{kT}}, \quad and \quad n(0) = N_C \cdot e^{-\frac{q\phi_B}{kT}}$$

$$J_{x} = \frac{qD_{n}N_{C}e^{-\frac{q\phi_{B}}{kT}}}{\int_{0}^{x_{d}}e^{-\frac{q\phi(x)}{kT}}dx} \times [e^{\frac{qV_{a}}{kT}} - 1]$$
 where  $\phi(x) = \frac{qN_{d}}{\varepsilon_{s}}\frac{x_{d}^{2}}{2}[1 - (1 - \frac{x}{x_{d}})^{2}]$ 

## **Surface States**

There are extra allowed states for electrons that are present at the semiconductor surface, but not within the bulk.

**Tamm or Shockley states** 

![](_page_50_Figure_3.jpeg)

Surface

![](_page_50_Figure_5.jpeg)

$$N_{st} \sim N_o^{2/3}$$
 (cm<sup>-2</sup>), for Si,  $N_o = 5 \times 10^{22}$  cm<sup>-3</sup>  
 $\longrightarrow N_{st} = 10^{15}$  cm<sup>-2</sup>

**Bonded foreign atoms or crystal defects** 

![](_page_50_Figure_8.jpeg)

- Donor states: states are neutral when occupied by electrons and positively charged when unoccupied.
- Acceptor states: states are negative when occupied and neutral when empty.

#### **Example:** Surface state and surface recombination velocity

An n-type Si wafer with a doping concentration of  $10^{18}$  cm<sup>-3</sup> at RT is illuminated through a passivating layer of SiO<sub>2</sub> so that the hole and electron density exceed their thermal equilibrium values. Assume that the surface electron density  $n_s = 10^{16}$  cm<sup>-3</sup> at thermal equilibrium, the photo generation of carriers is  $2 \times 10^{14}$  cm<sup>-2</sup>s<sup>-1</sup>, and the surface hole density under illumination increases to  $p_s = 10^{10}$  cm<sup>-3</sup>.

![](_page_51_Figure_2.jpeg)

Since  $n_{so} = 10^{16}$  cm<sup>-3</sup> <<  $N_d = 10^{18}$  cm<sup>-3</sup>, the surface is slightly depleted of majority carriers.

The thermal equilibrium density of hole is

 $p_{so} = n_i^2 / n_{so} = 2.1 \times 10^4$ 

After photo generation,

 $p_s = 10^{10} \text{ cm}^{-3} >> p_{so},$ 

therefore the excess carrier density of hole is  $\Delta p_s = 10^{10} \text{ cm}^{-3}$ 

If  $S_p = 10^4$  cm/s, the net recombination rate is

 $U_s = S_p \times \Delta p_s = 10^{14} \text{ cm}^{-2} \text{s}^{-1},$ 

therefore 50% of the excess carriers are recombined at the surface.

# **Part II – Optics**

## **Maxwell's equations and wave propagation**

Maxwell's equations, in MKS unit, can be written in the form

$$\nabla \times \vec{E}(\vec{r},\omega) = -\frac{\partial \vec{B}}{\partial t} \quad \nabla \times \vec{H}(\vec{r},\omega) = \vec{J} + \frac{\partial \vec{D}}{\partial t} \quad \nabla \cdot \vec{B} = 0 \quad and \quad \nabla \cdot \vec{H} = \rho$$
  
$$\vec{E} : V/m \quad \vec{H} : A/m \qquad \vec{B} : \frac{V \cdot \sec}{m^2} = \frac{Web}{m^2} \quad \vec{D} : \frac{C}{m^2} \quad \rho : \frac{C}{m^3} \quad and \qquad \vec{J} : \frac{A}{m^2}$$
  
Continuity equation: 
$$\nabla \cdot \vec{J}(\vec{r},\omega) = -\frac{\partial \rho}{\partial t}$$

Totally, we have 15 unknowns, but with only 6 independent equations. To solve the Maxwell's equations, we need more equations.

## Constitutive relation

$$\begin{split} \vec{J}(\vec{r},\omega) &= f\{\vec{E}(\vec{r},\omega), \vec{B}(\vec{r},\omega)\} \quad \vec{D}(\vec{r},\omega) = f\{\vec{E}(\vec{r},\omega), \vec{B}(\vec{r},\omega)\} \quad and \\ \vec{H}(\vec{r},\omega) &= f\{\vec{E}(\vec{r},\omega), \vec{B}(\vec{r},\omega)\} \end{split}$$

In a linear lossless, homogeneous, and isotropic medium, the constitutive relation can be written as

$$\overline{J}(\overline{r},\omega) = 0$$
  $\overline{D}(\overline{r},\omega) = \varepsilon(\omega)\overline{E}(\overline{r},\omega)$  and  $\overline{H}(\overline{r},\omega) = \frac{\overline{B}(\overline{r},\omega)}{\mu(\omega)}$ 

**Additional 6 equations** 

## **Monochromatic plane waves**

Consider a homogenous and source free region in free space, then

 $\vec{J}(\vec{r},\omega) = 0$   $\vec{D}(\vec{r},\omega) = \varepsilon_0 \vec{E}(\vec{r},\omega)$   $\vec{B}(\vec{r},\omega) = \mu_0 \vec{H}(\vec{r},\omega)$ 

For a monochromatic plane wave,

$$\vec{E}(\vec{r},\omega) = \operatorname{Re}[\vec{E}(\vec{r})e^{-i\omega t}] \quad and \quad \vec{H}(\vec{r},\omega) = \operatorname{Re}[\vec{H}(\vec{r})e^{-i\omega t}]$$

$$\Rightarrow \quad \nabla \times \vec{E} = i\omega\mu_0 \vec{H} \quad \nabla \times \vec{H} = -i\omega\varepsilon_0 \vec{E} \quad and \quad \nabla \cdot \vec{E} = \nabla \cdot \vec{H} = 0$$

Consider now,

$$\nabla \times \nabla \times \vec{E} = \nabla (\nabla \cdot \vec{E}) - \nabla^2 \vec{E} = i\omega\mu_0 \nabla \times \vec{H} = \omega^2 \mu_0 \varepsilon_0 \vec{H}$$
  

$$\bigcirc \quad \nabla^2 \vec{E} + k^2 \vec{E} = 0 \quad \nabla^2 \vec{H} + k^2 \vec{H} = 0 \quad and \quad k^2 = \omega^2 \mu_0 \varepsilon_0 = \omega^2 c^2$$
  
Wave equations

The solutions to above wave equations can be written as

$$\vec{E} = \vec{E}_{f}e^{i\vec{k}\cdot\vec{r}} + \vec{E}_{b}e^{-i\vec{k}\cdot\vec{r}} \quad and \quad \vec{H} = \vec{H}_{f}e^{i\vec{k}\cdot\vec{r}} + \vec{H}_{b}e^{-i\vec{k}\cdot\vec{r}} \quad \text{or}$$
$$\vec{E}(\vec{r},t) = \vec{E}_{f}\cos(\omega t - \vec{k}\cdot\vec{r}) + \vec{E}_{b}\cos(\omega t + \vec{k}\cdot\vec{r})$$
$$Phase functions$$

If we only consider the forward-propagating waves,

$$\vec{E} = \vec{E}_{f} e^{i\vec{k}\cdot\vec{r}}$$
 and  $\vec{H} = \vec{H}_{f} e^{i\vec{k}\cdot\vec{r}}$ 

Use 
$$\nabla \times \vec{E} = i\omega\mu_0 \vec{H}$$
  
 $i\vec{k} \times \vec{E}_f e^{i\vec{k}\cdot\vec{r}} = i\omega\mu_0 \vec{H}_f e^{i\vec{k}\cdot\vec{r}} \rightarrow \frac{\vec{k}}{k} \times \vec{E}_f = \sqrt{\frac{\mu_0}{\varepsilon_0}} \vec{H}_f \rightarrow \hat{e}_k \times \vec{E}_f = \sqrt{\frac{\mu_0}{\varepsilon_0}} \vec{H}_f = \eta_0 \vec{H}_f$   
Similarly,  $\hat{e}_k \times \vec{H}_f = -\frac{1}{\eta_0} \vec{E}_f$  and  $\hat{e}_k \cdot \vec{H}_f = \hat{e}_k \cdot \vec{E}_f = 0$   
 $\vec{E}_f$   
 $\vec{H}_f$  and  $|E_f| = \eta_0 |H_f|$ 

\_\_\_\_

Consider now, if the wave is propagating along z direction

![](_page_56_Figure_2.jpeg)

 $|E_x| = \eta_0 |H_y| : x - polarized$  and  $|E_y| = -\eta_0 |H_x| : y - polarized$ 

### **Example:** Plane waves

What is a plane wave?

The wave has a perfect flat and infinite in extent phase front.

So under what condition, an obtainable wave can be approximated as a plane wave?

![](_page_57_Figure_4.jpeg)

**Does not exit!** 

Let the truncated x-polarized wave be  $\vec{E} = \hat{e}_x E_x e^{ik \cdot z} e^{-\frac{r^2}{2w_o^2}}$   $w_o: beam\_waist$ 

For such a plane wave,  $E_y = H_x = E_z = H_z = 0$ , and  $E_x = \eta H_y$ 

However, we always have 
$$\nabla \cdot \vec{E} = 0 = \frac{\partial E_x}{\partial x} + \frac{\partial E_y}{\partial y} + \frac{\partial E_z}{\partial z}$$
  
If the wave is truncated,  $\frac{\partial E_x}{\partial x} \neq 0$ 

 $\overrightarrow{E} = \hat{e}_x E_x + \hat{e}_z E_z \quad and \quad \overrightarrow{H} = \hat{e}_y H_y + \hat{e}_z H_z$ 

Consider the Poynting vector,  $\vec{S} = \vec{E} \times \vec{H} = \hat{e}_z E_x H_y - \hat{e}_y E_z H_z - \hat{e}_z E_z H_y$ 

There must be radial components of the Poynting vector. This effect is also know as diffraction spreading.

![](_page_58_Figure_4.jpeg)

## **Polarization**

Assuming a plane wave propagating along z direction,

$$\bar{E}_{t} = \hat{e}_{x}E_{x}(\vec{r},t) + \hat{e}_{y}E_{y}(\vec{r},t)$$
  
and  $E_{x}(\vec{r},t) = a_{x}\cos(\omega t - kz + \varphi_{x})$   $E_{y}(\vec{r},t) = a_{y}\cos(\omega t - kz + \varphi_{y})$ 

Let  $\tau = \omega t - kz$ , then

$$\frac{E_x}{a_x} = \cos\tau \cdot \cos\varphi_x - \sin\tau \cdot \sin\varphi_x \quad and \quad \frac{E_y}{a_y} = \cos\tau \cdot \cos\varphi_y - \sin\tau \cdot \sin\varphi_y$$

Eliminating  $\tau$  from above equation,

$$(\frac{E_x}{a_x})^2 + (\frac{E_y}{a_y})^2 - 2\frac{E_x E_y}{a_x a_y} \cos \varphi = \sin^2 \varphi \quad and \quad \varphi = \varphi_x - \varphi_y$$

## **Example:** Polarization

$$\left(\frac{E_x}{a_x}\right)^2 + \left(\frac{E_y}{a_y}\right)^2 - 2\frac{E_x E_y}{a_x a_y}\cos\varphi = \sin^2\varphi \quad and \quad \varphi = \varphi_x - \varphi_y$$

![](_page_60_Figure_2.jpeg)

![](_page_60_Figure_3.jpeg)

![](_page_60_Figure_4.jpeg)

![](_page_60_Picture_5.jpeg)

![](_page_60_Figure_6.jpeg)

![](_page_60_Figure_7.jpeg)

![](_page_60_Picture_8.jpeg)

## **Detection**

![](_page_61_Figure_1.jpeg)

$$\vec{S} = \vec{E} \times \vec{H} = \hat{e}_{z} \{ \frac{a_{1}^{2}}{2\eta_{0}} [1 + \cos(2\omega t - 2kz)] + \frac{a_{2}^{2}}{2\eta_{0}} [1 + \cos(2\omega t - 2kz + 2\varphi)] \}$$

So energy flows of the two polarization states simply add up together and no cross terms.

![](_page_61_Figure_4.jpeg)

Since no detector can react fast enough at optical frequency, so what we actually see is the average energy across A.

$$\vec{S} = \vec{E} \times \vec{H} = \hat{e}_{z} \{ \frac{a_{1}^{2}}{2\eta_{0}} [1 + \cos(2\omega t - 2kz)] + \frac{a_{2}^{2}}{2\eta_{0}} [1 + \cos(2\omega t - 2kz + 2\varphi)] \}$$
  
Take < >,

$$\langle \vec{S}(z,t) \rangle = \frac{1}{2\tau_d} \int_{t-\tau_d}^{t+\tau_d} \vec{S}(z,t) dt \quad \tau_d : \det ector\_response\_time$$

Since  $\tau_d >> T_{opt}$ , so the response time average ~ infinite time average.

$$<\bar{S}(z,t)>=\lim \frac{1}{2T}\int_{-T}^{T}\bar{S}(z,t)dt=(\frac{a_{1}^{2}}{2\eta_{0}}+\frac{a_{2}^{2}}{2\eta_{0}})\hat{e}_{z}$$

Therefore the energy flow is directly proportional to the time average of  $\vec{E}(t) \cdot \vec{E}(t)$ .

$$S_{ave} = \langle S(t) \rangle = \frac{1}{2} \operatorname{Re}(\vec{E} \times \vec{H}^*) = \frac{1}{2} EH^* = \frac{E^2}{2\eta_0}$$

#### **Example:** Transmission and reflection coefficients

![](_page_63_Figure_1.jpeg)

Note that  $R + T \xrightarrow{TE} |r_{\perp}|^2 + |t_{\perp}|^2 = \frac{5n_1 - 2n_1n_2 + n_2^2}{(n_1 + n_2)^2} = 1_{only\_if\_n1=n2}$ 

## **Brewster angle**

![](_page_64_Figure_1.jpeg)

Therefore there must exist the condition, when  $\theta_1 = \theta_B$  $\rightarrow \theta_1 = \theta_r \rightarrow \theta_r + \theta_2 = \pi/2 \rightarrow tan\theta_B = n_2/n_1$ 

So when  $\theta_1 = \theta_B \rightarrow r_{//} = 0$ , indicating no reflection and total transmission.

## **Total internal reflection (TIR)**

![](_page_65_Figure_1.jpeg)

**Snell's law:**  $n_1 \sin \theta_i = n_2 \sin \theta_i$   $n_1 > n_2$ Increasing  $\theta_i$  will also increase  $\theta_t$ . When  $\theta_i = \theta_{i2} = \theta_c \rightarrow \theta_{f2} = 90^\circ, \text{ or }$  $n_{1} \sin \theta_{i2} = n_{2} \quad \Rightarrow \quad \theta_{i2} \equiv \theta_{c} = \sin^{-1} \frac{n_{2}}{n_{1}}$ If  $\theta_{i} > \theta_{c}$ ,  $n_{1} \sin \theta_{i} = n_{2} \sin \theta_{t}$  or  $\sin \theta_{t} = \frac{n_{1}}{n_{2}} \sin \theta_{i} > 1$  $\vec{k}_{1x} = \vec{k}_{2x}$  Snell'\_law and  $\vec{k}_{2}^{2} = \vec{k}_{2x}^{2} + \vec{k}_{2z}^{2} = \vec{k}_{1x}^{2} + \vec{k}_{2z}^{2} = \vec{k}_{1}^{2} \sin^{2}\theta_{i} + \vec{k}_{2z}^{2}$  $\Rightarrow \quad \vec{k}_{2z}^2 = \vec{k}_2^2 - \vec{k}_1^2 \sin^2 \theta_i = \omega^2 \mu \varepsilon_2 - \omega^2 \mu \varepsilon_1 \sin^2 \theta_i = \omega^2 \mu \varepsilon_2 [1 - (\frac{n_1}{n_2} \sin \theta_i)^2]$  $k_{2z} = -i\omega\sqrt{\mu\varepsilon_2}\sqrt{(\frac{n_1}{n_2}\sin\theta_i)^2 - 1} = -ik_2\sqrt{(\frac{n_1}{n_2}\sin\theta_i)^2 - 1}$ 

## **Example:** Evanescence waves in z direction

$$\vec{E}_{t}^{TE} = t \times \vec{E}_{i} e^{i\omega t} e^{-i\vec{k}\cdot\vec{r}} = t \times \vec{E}_{i} e^{i\omega t} e^{-ik_{2x}\cdot x} e^{-ik_{2z}\cdot z} \quad \text{Since} \quad k_{2z} = -ik_{2}\sqrt{\left(\frac{n_{1}}{n_{2}}\sin\theta_{i}\right)^{2} - 1}$$

$$= t \times E_{i} e^{i\omega t} e^{ik_{2x}x\sin\theta_{t}} e^{-k_{2}\sqrt{(\sin^{2}\theta_{t}-1)z}} \quad \text{or} \quad \rho = \frac{\lambda_{2}}{2\pi} \frac{1}{\sqrt{(\sin^{2}\theta_{t}-1)}}$$

$$= t \times E_{i} e^{i\omega t} e^{ik_{2x}x\sin\theta_{t}} e^{-k_{2}\sqrt{(\sin^{2}\theta_{t}-1)z}} \quad \text{or} \quad \rho = \frac{\lambda_{2}}{2\pi} \frac{1}{\sqrt{(\sin^{2}\theta_{t}-1)}}$$

$$\text{Propagating Evanescent wave} \quad \text{Goos-Hanschen depth}$$

So we have a propagating wave along x direction (real  $k_{1x} = k_{2x}$ ) and an evanescent wave along z direction (imaginary  $k_{2z}$ ).

$$\uparrow_{\rho}$$

## **Example: TIR** applications

#### I. Circular polarization

![](_page_67_Figure_2.jpeg)

II. Prism coupler

#### **III. Optical waveguide**

![](_page_67_Figure_5.jpeg)

![](_page_67_Figure_6.jpeg)