Chapter X: Interfaces between Dissimilar materials and Heterostructures

X.1.Introduction

In semiconductor physics, several types of material junctions exist:

- **Homo-junction**: contact between differently doped regions of the same semiconductor (e.g., PN junctions).
- **Hetero-junction**: interface between two different semiconductors.
- **Metal-Semiconductor contact**: forms either Schottky or ohmic contacts.
- **MIS structure**: Metal–Insulator–Semiconductor, often realized as **MOS** (with oxide as the insulator).

When two different materials come into contact—such as a metal and a semiconductor, or two distinct semiconductors—their electrical properties at the interface differ significantly from those of the individual materials. These interfaces play a crucial role in modern electronic and optoelectronic devices. This chapter explores the physical mechanisms governing these contacts, focusing on metal–semiconductor interfaces and heterojunctions between semiconductors.

Understanding these contacts requires key concepts such as work function, electron affinity, and potential barriers.

X.2. Work function – Electron affinity – Potential barrier

X.2.1. Work function

- In a **metal**:

- the **work function (ΦM)** is the energy needed to remove an electron from the Fermi level E_{FM} to the vacuum level E_0:

$$\Phi_M = E_0 - E_{FM}$$

- In a **semiconductor:**

- the **work function** (**ΦSC**) is defined as the energy difference between the vacuum level and the Fermi level E_{FSC} in the semiconductor.

$$\Phi_{SC} = E_0 - E_{FSC}$$

X.2.2. Electron affinity

the **electron affinity (χ)** is the energy required to remove a "free" electron from the conduction band minimum to vacuum level:

$$\chi = E_0 - E_C$$

Typical electron affinity values are:

- $\chi \approx 4\ eV$ for Si, GaAs, Ge
- $\chi \approx 1.1\ eV$ for SiO_2 (insulating oxide)

- The **Schottky barrier height (ΦB)** defines the energy barrier electrons face from metal to semiconductor:

$$\Phi_B = \Phi_M - \chi = E_C - E_{FM}$$

This is known as the **Schottky–Mott rule**. It indicates that the barrier depends on both the metal's work function and the semiconductor's electron affinity.

X.2.3. Barrier formation and band bending

At equilibrium, the Fermi level aligns across the metal–semiconductor structure, leading to:

- Electrons may flow from the semiconductor to the metal or vice versa.

- This results in **band bending** and the formation of a **space charge region (SCR)** in the semiconductor.
- The metal side, having a very high carrier density, shows negligible band bending.

The resulting band diagram shows:

- Upward bending of the conduction and valence bands in the semiconductor (for Schottky contact).
- A **built-in potential** V_S across the depletion region, representing the energy barrier for carriers in the semiconductor to reach the metal:

$$-qV_S = \Phi_B - (E_C - E_{FSC}) = \Phi_M - \Phi_{SC}$$

The figure below shows the Energy-band diagrams of metal – semiconductor junctions before and after contact:

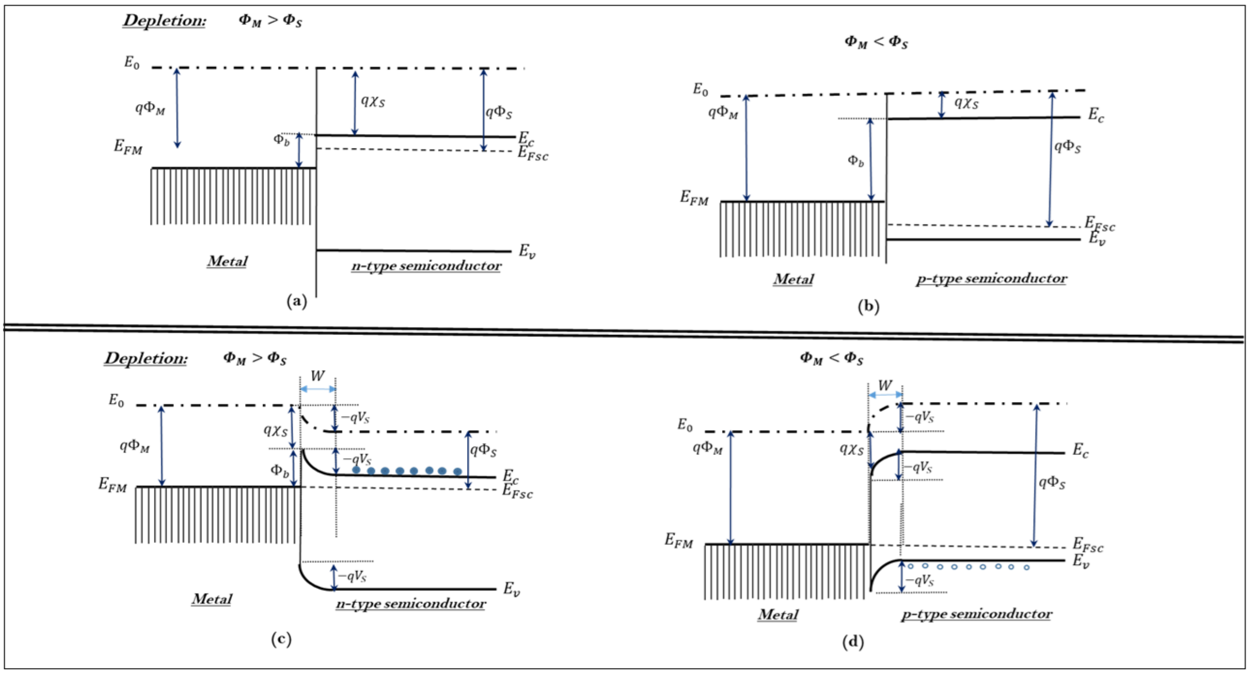

Figure X.1. Energy-band diagrams of metal – semiconductor junctions: (a,b) before contact with n-type and p-type semiconductors, respectively; (c,d) after contact with n-type and p-type semiconductors.

X.3. Real Metal-Semiconductor contact

I.3.1. Native Oxide Layer

A thin oxide (10–20 Å) often exists between the metal and semiconductor. Electrons can still tunnel through it, but it modifies the barrier height. The oxide acts like a capacitor, influencing the surface potential.

- Modified surface potential:

$$-qV_S = \Phi_M - \Phi_{SC} + qV_{OX}$$

Where $\mathbf{V_{OX}}$ represents a voltage across oxide.

- Modified Schottky barrier:

$$\Phi_B = \Phi_M - \chi + qV_{OX}$$

This native oxide behaves like a **parallel-plate capacitor**, where the charge on the metal side Q_M is equal and opposite to the sum of charges in the semiconductor Q_{SC}:

$V_{OX} = \frac{Q_M}{C_{OX}}$, with $C_{OX} = \frac{\varepsilon_{OX}}{t_{OX}}$

Where:

- C_{OX} is the oxide capacitance per unit area,
- ε_{OX} is the permittivity of the oxide,
- t_{OX} is its thickness.

Such corrections are especially relevant for **ionic semiconductors** (e.g., ZnS, ZnO, AlN), where high-quality surfaces make this model accurate. Nevertheless, the barrier height still shows some **dependence on the metal**, contrary to what this model might predict in certain cases.

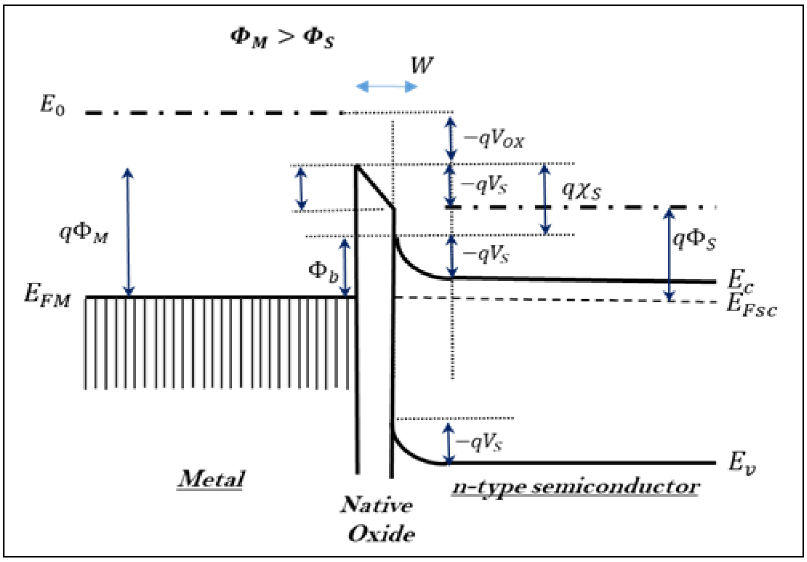

Figure X. 2 Metal/Semiconductor contact with oxide layer after contact

X.3.2. Interface states

Imperfect semiconductor surfaces can trap electrons or holes—these are called **interface states**. They behave like donor or acceptor levels and strongly affect the barrier height. In some cases, the barrier becomes almost independent of the metal (Bardeen limit).

The occupation probability of an interface state at energy E_t:

$$f(E_t) = \frac{1}{1 + e^{\frac{E_t - E_{FSC}}{KT}}}$$

The **total interface charge Q**ss contributes to the balance:

$$\Phi_M = -(\Phi_{SC} + \Phi_{SS})$$

If interface states are dense, they "pin" the Fermi level, and the barrier becomes almost independent of the metal (Bardeen limit). Then:

$$\Phi_B \approx \frac{2}{3} E_g$$

Table X.1. Summary of Key Effects in Real Contacts

Effect	Cause	Consequence
Native oxide layer	Spontaneous surface oxidation	Creates additional potential drop V_{OX}
Interface states	Surface defects, dangling bonds, contamination	Capture/release carriers, modify barrier height
Fermi level pinning (Bardeen)	High density of interface states	Φ_B independent of metal work function
Charge redistribution	Equilibrium condition	Band bending, depletion region, surface potential

X.4. Metal–Semiconductor contact, I – V Qualitative behavior

The electrical behavior of a metal–semiconductor (M–S) contact depends on how charge carriers move across the junction. Depending on the barrier properties and doping level, the contact may behave as a **diode (rectifying)** or a **resistor (ohmic)**.

X.4.1. Rectifying Contact (Schottky Diode)

In an **n-type SC**, with $\Phi_M > \Phi_{SC}$, a depletion region forms. The current is due to majority carriers (electrons).

At thermal equilibrium (no applied voltage), the two electron flows (metal ↔ SC) cancel, so

$$I = 0$$

With an applied bias V, the current becomes:

$$I = I_S(e^{\frac{qV}{KT}} - 1)$$

Where I_S is the reverse saturation current.

The Schottky diode allows current mostly in one direction:

- **Forward bias $V > 0$:**

$$I \approx I_S e^{\frac{qV}{KT}}$$

electrons move from semiconductor to metal. Barrier lowers and current increase exponentially.g

- **Reverse bias $V < 0$**: Barrier increase and only a small saturation current flows:

$I \approx -I_S$ (independent of V)

Schottky diodes are fast and efficient due to majority carrier transport and low forward voltage.

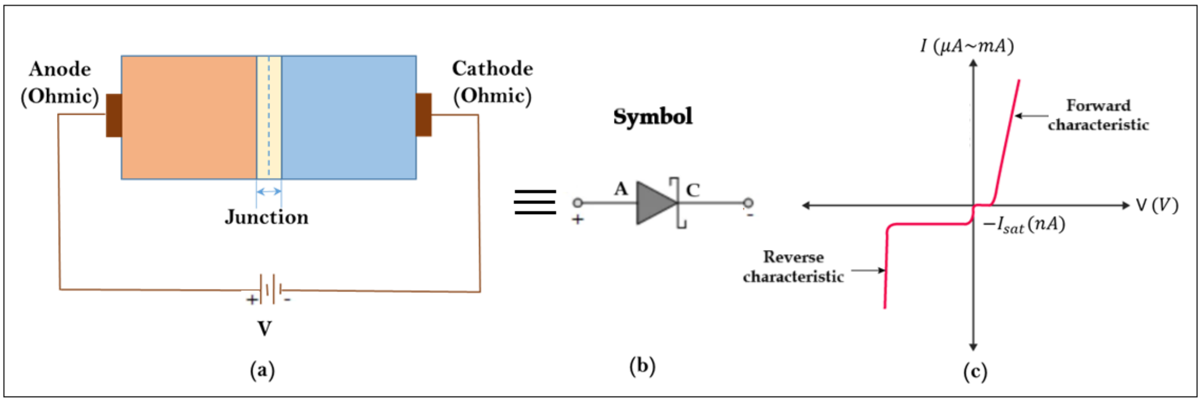

Figure X.3 Metal/Semiconductor contact (Schottky Diode): (a)Junction M-SC, (b) Symbol, (c) I–V relationship

X.4.2. Ohmic contact

Occurs when the interface **does not block carriers**. For instance, if the SC is **heavily doped**, the barrier is thin and tunneling dominates, or the interface forms an **accumulation region**.

The current–voltage relationship is linear: $I = \frac{V}{R}$

Where $\boldsymbol{R}$ is the contact resistance, often dominated by the neutral SC region.

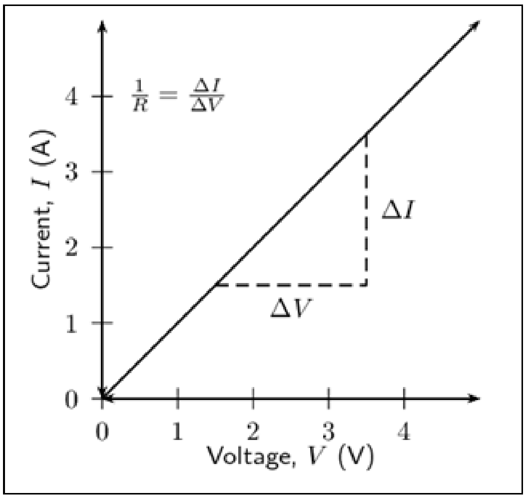

Figure X.4 Ohm's Law

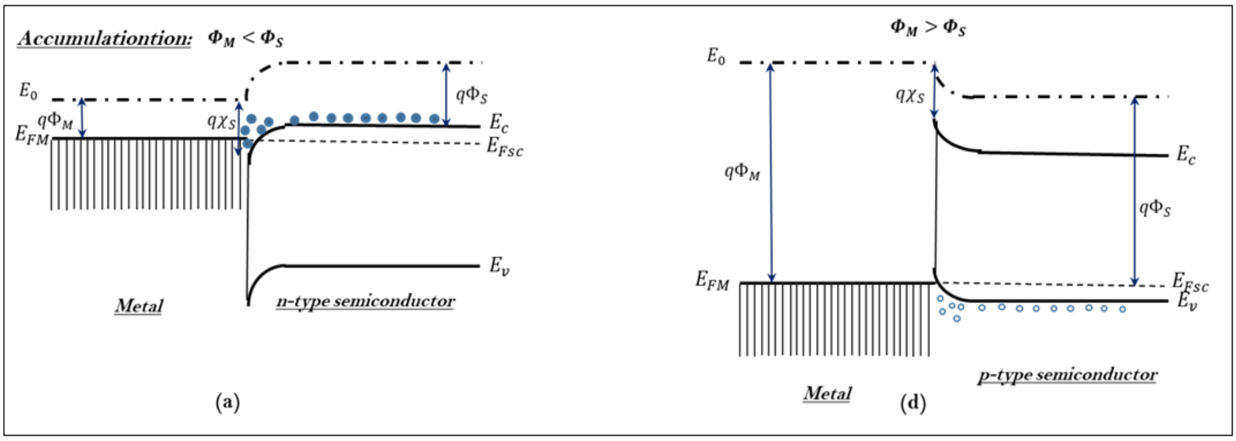

Figure X.5 Ohmic contact with accumulation SCR

Table X.2. Summary: Schottky vs. ohmic contacts

Property	**Schottky contact**	**Ohmic contact**
Barrier shape	Rectifying (depletion region)	Linear/resistive (accumulation or tunneling)
I-V characteristic	Exponential in forward, suturing in reverse	Linear (Ohm's Law)
Carrier type	Majority carriers only	Majority carriers only

Band bending	Depletion region	Accumulation or tunneling
Reverse saturation	Hign	Not applicable
Switching speed	Very fast	Fast (but depends on resistance)
Doping level required	Moderate (n or p)	Very high (degenerate n+ or p+)
Application	Diodes, fast switching	Electrical contacts (interconnects)

X.5. Heterojunction

A **heterojunction** is a junction between two **different semiconductor materials**.

- If both semiconductors are of the **same type** (both *n-type* or both *p-type*), the junction is called an **isotype heterojunction**.
- If they are of **different types** (*p-type* and *n-type*), it is called an **anisotype heterojunction**.

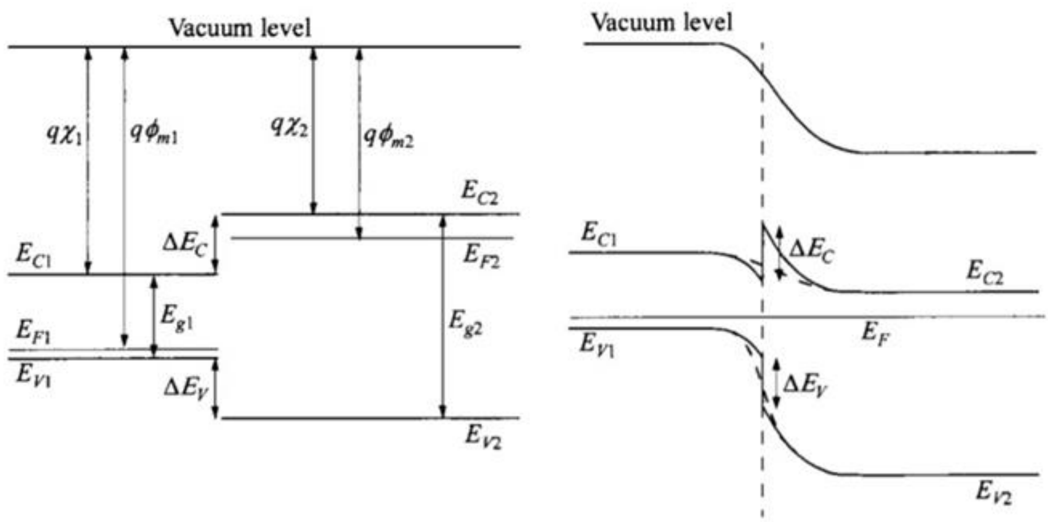

Figure X.6 P-n heterojunction formation. Energy bands diagram of two different semiconductors before (left), and after the merge (right).

Heterojunctions are the basis for **high-performance devices**, especially in **high-frequency** and **optoelectronic** applications, such as:

- HEMTs (High Electron Mobility Transistors),
- HBTs (Heterojunction Bipolar Transistors),
- LEDs and **laser diodes**.

X.5.1. Energy band diagram

A **heterojunction** is the contact between two different semiconductors. It introduces **discontinuities** in the conduction and valence bands (or conduction and valence bands offset): ΔE_C and ΔE_V, which control how electrons and holes move across the junction.

Three types of heterojunction exist:

- **Type I (Straddling gap)**: Electrons and holes are confined in the same material.

  $E_{C1} > E_{C2}$, $E_{V1} < E_{V2}$.

- **Type II (Staggered gap)**:

  $E_{C1} > E_{C2}$, $E_{V1} > E_{V2}$.

  Electrons and holes are separated spatially.

- **Type III (Broken gap)**:

  $E_{V1} > E_{C2}$

One band overlaps with the opposite type in the other material.

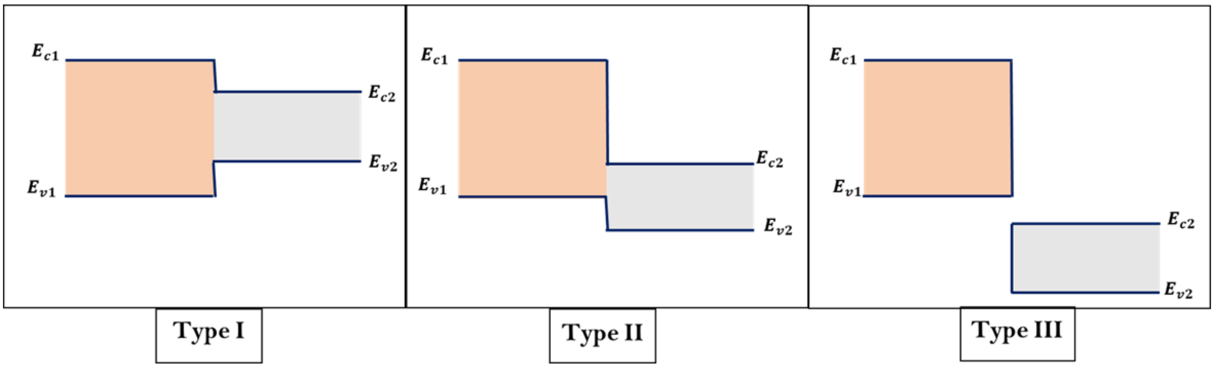

Figure X.7. **Three possible types of heterojunction: straddling gap (type I), staggered gap (type II), broken gap (type III).**

X.5.2. Applications: carrier localization and transport

Heterojunctions are widely used to control where carriers are located:

- **Quantum wells**:

electrons (and/or holes) are trapped in narrow regions where energy levels become quantized.

- **Optoelectronic devices**: e.g., **LEDs and lasers**:

where confined carriers recombine to emit light.

- **High-Electron Mobility Transistors (HEMTs)**: .

  - 2D electron gas forms at the heterointerface,
  - High mobility due to minimal impurity scattering

- **HBT (Heterojunction Bipolar Transistor)**:

Uses barriers to allow injection of one carrier type and block the other.

In many cases, heterojunctions are designed to allow one carrier type to cross the junction easily while blocking the other. This selective behavior is key in devices like **heterojunction bipolar transistors (HBTs)** and **hot electron devices**.