



# CHARGE TRANSPORT ACROSS METAL N-TYPE SEMICONDUCTOR INTERFACES.

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# Abstract

In this study, we considered the thermionic emission, field emission and tunneling and we derived current density as a functions of different parameters such as, temperature, barrier height, work function, bias voltage and dopant concentration for thermionic emission, field emission and tunneling enhanced electron transport across metal and N-type semiconductor interfaces.

The result shows that the thermionic current density is increasing exponentially as a functions of bias voltage, the current density is also increasing as a quadratic functions of temperature and current density is increasing linearly as a functions of dopant concentration. Therefore, we carry out investigation how these factors affect the current density and we solve the current density analytically with a given parameters. The results are plotted using gnuplot.

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# Chapter 1

## INTRODUCTION

Formation of electronic devices requires putting together two or more dissimilar materials (semiconductors, metals, insulators). The interface between these materials becomes crucial because it affects the electrical properties (transport) of the devices. This interface is called a junction. An ideal junction is one where there are no defects formed at the interface. Forming ideal junctions is challenging and most real materials have defects at the interface which can affect the electronic properties. But we can get an idea of an interaction between materials by studying ideal junction[1].

### 1.1 Schottky junctions

When a metal and semiconductor are brought into contact, there are two types of junctions formed depending on the work function of the semiconductor and its relation with the metal

1. Schottky junction when  $\phi_m > \phi_{semi}$
2. Ohmic junction when  $\phi_m < \phi_{semi}$

Consider a junction formed between a metal and n-type semiconductor, The Fermi level of the semiconductor is higher (since its work function is lower) than the metal. Similar to a metal-metal junction, when the metal-semiconductor junction is formed the Fermi levels must line up at equilibrium. Another way to look at this is that

there are electrons in the conduction band of the semiconductor which can move to the empty energy states above the Fermi level of the metal. This leaves a positive charge on the semiconductor side and due to the excess electrons, a negative charge on the metal side, leading to a contact potential[3]. when a contact is formed between a metal and semiconductor, due to the low charge density on the semiconductor side (typically  $10^{17}cm^{-3}$ ) the electrons are removed not only from the surface interaction between materials by studying ideal junction, but also from a certain depth within the semiconductor. This leads to the formation of a depletion region within the semiconductor. Thus, when a Schottky junction is formed between the metal and semiconductor, the Fermi level lines up and also a positive potential is formed on the semiconductor side. Because the depletion region extends within a certain depth in the semiconductor there is bending of the energy bands on the semi-conductor side. Bands bend up in the direction of the electric field from positive charge to negative charge, opposite of the potential direction. This means the energy bands bend up going from n-type semiconductor to Metal. The Fermi levels line up and there is a certain region in the semiconductor (denoted by W), where the bands bend (this is the depletion region). Another name for the depletion region is the space charge layer. There is a built in potential in the Schottky junction which is given by the difference in work functions. [2]

$$eV_o = \phi_m - \phi_{semi} \quad (1.1.1)$$

The work function of the metal is a constant while that of the semiconductor work function depends on the dopant concentration (since this affects the Fermi level position). The contact potential then represents the barrier for the electrons to move from the n-type semiconductor to the metal. Initially, when the junction is formed electrons move to the metal and create the depletion region in the semiconductor. The contact potential thus formed prevents further motion of the electrons to the metal. There is also a barrier for electrons to move from the metal to semiconductor.

This is called a Schottky barrier.

## 1.2 Formation of Barrier

When a metal makes contact with a semiconductor, a barrier is formed at the metal semiconductor interface. This barrier is responsible for controlling the current conduction as well as its capacitance behavior. At equilibrium the motion of electrons from the semiconductor to metal is balanced by the contact potential so that there is no net current. The Schottky junction can be biased by application of an external potential[3]. There are two types of bias

1. Forward bias - metal is connected to positive terminal and n-type semi-conductor connected to negative terminal.
2. Reverse bias - metal is connected to negative terminal and n-type semi-conductor connected to positive terminal. The current flow depends on the type of bias and the amount of applied external potential.

## 1.3 Forward bias

In a forward biased Schottky junction the external potential is applied in such a way that it opposes the in-built potential. Since the region with the highest resistivity is the depletion region near the junction, the voltage drop is across the depletion region. Under external bias the Fermi levels no longer line up, but are shifted with respect to one another and the magnitude of the shift depends on the applied voltage. Thus, electrons injected from the external circuit into the n-type semiconductor have a lower barrier to surmount before reaching the metal. This leads to a current in the circuit which increases with increasing external potential. The current in a Schottky diode under forward bias is given by

$$J = J_o[\exp(\frac{ev}{k_B T}) - 1] \quad (1.3.1)$$

where  $J$  is the current

$e$  is charges of electron

$V$  is applied voltage and  $J_o$  is thermionic current

## 1.4 Ideal Condition

The electronic energy relations of a high work-function metal and n-type semiconductor which are not in contact and are in separate systems. If metal and n-type semiconductor are allowed to communicate with each other, for example by an external wire connection, charge will flow from the semiconductor to the metal and thermal equilibrium is established as a single system. The Fermi levels on both sides will line up. Relative to the Fermi level in the metal, the Fermi level in the semiconductor is lowered by an amount equal to the difference between the two work functions. The work function is the energy difference between the vacuum level and the Fermi level. This quantity is denoted by  $q\phi_m$  for the metal, and is equal to  $q(x + \phi_n)$  in the semiconductor, where  $q\phi_x$  is the electron affinity measured from the bottom of the conduction band  $E_c$ , to the vacuum level, and  $q\phi_n$  is the energy difference between  $E_c$  and the Fermi level. The potential difference between the two work functions is called the contact potential. As the gap distance  $\delta$  decreases, the electric field in the gap increases and an increasing negative charge is built up at the metal surface. An equal and opposite charge (positive) must exist in the semiconductor depletion region. The potential variation within the depletion layer is similar to that in one side of a p-n junction. When  $\delta$  is small enough to be comparable to the interatomic distances, the gap becomes transparent to electrons, and we obtain the limiting. It is clear that the limiting value of the barrier height is given by  $q\phi_{Bno} = q(\phi_m - \chi)$ . where  $\chi$  is electron affinity The barrier height is simply the difference between the metal work function and the electron affinity of the semiconductor.

## Chapter 2

# CURRENT TRANSPORT PROCESSES

The current transport in metal-semiconductor contacts is due mainly to majority carriers, in contrast to p-n junctions where the minority carriers are responsible. There are five basic transport processes under forward bias (the inverse processes occur under reverse bias). These five processes are

1. emission of electrons from the semiconductor over the potential barrier into the metal [the dominant process for Schottky diodes with moderately doped semiconductors (e.g., Si with  $N_D \leq 10^{17} \text{cm}^{-3}$ ) operated at moderate temperatures (e.g., 300K)],
2. quantum mechanical tunneling of electrons through the barrier (important for heavily doped semiconductors and responsible for most ohmic contacts)
3. recombination in the space-charge region [identical to the recombination process.
4. diffusion of electrons in the depletion region, and
5. holes injected from the metal that diffuse into the semiconductor (equivalent to recombination in the neutral region). In addition, we may have edge leakage current due to a high electric field at the metal-contact periphery or interface current due to traps at the metal-semiconductor interface. For common high-mobility semiconductors (e.g. Si and GaAs) the transport can be adequately described by this thermionic-emission theory. We shall also consider the diffusion theory applicable to

low-mobility semiconductors and a generalized thermionic-emission-diffusion theory that is a synthesis of the preceding two theories. Schottky diode behavior is to some extent electrically similar to a one-sided abrupt p-n junction, and yet the Schottky diode can be operated as a majority-carrier device with inherent fast response. Thus, the terminal functions of a p-n junction diode can general be performed by a Schottky diode with one exception as a charge storage diode. This is because the charge-storage time in a majority-carrier device is extremely small. Another difference is the larger current density in a Schottky diode due to the smaller built-in potential as well as the nature of thermionic emission compared to diffusion. This results in a much smaller forward voltage drop. By the same token, the disadvantage is the larger reverse current in the Schottky diode and a lower breakdown voltage.

## 2.1 Depletion Layer

The depletion layer of a metal-semiconductor contact is similar to that of the one sided abrupt (e.g.  $p^+ - n$ ) junction. It is clear from the discussion above that when a metal is brought into intimate contact with a semiconductor, the conduction and valence bands of the semiconductor at the surface are brought into a definite energy relationship with the Fermi level in the metal. Once this relationship is established, it serves as a boundary condition to the solution of the Poisson equation in the semiconductor, which proceeds in exactly the same manner as in a p-n junction. For contacts on n-type semiconductors, under the abrupt approximation that charge density  $\rho \simeq qN_D$  for  $x < W_D$ ,  $\rho \simeq 0$  and  $E \simeq 0$  for  $x > W_D$ , The one dimensional poisson equation in the depletion of schottky diode is given by

$$\frac{d^2v(x)}{dx^2} = \frac{-\rho}{\epsilon_s} \quad (2.1.1)$$

by integrating the above equation

$$E(x) = \frac{-dv(x)}{dx} = \left(\frac{qN_D}{\epsilon_s}\right)x + c_1 \quad (2.1.2)$$

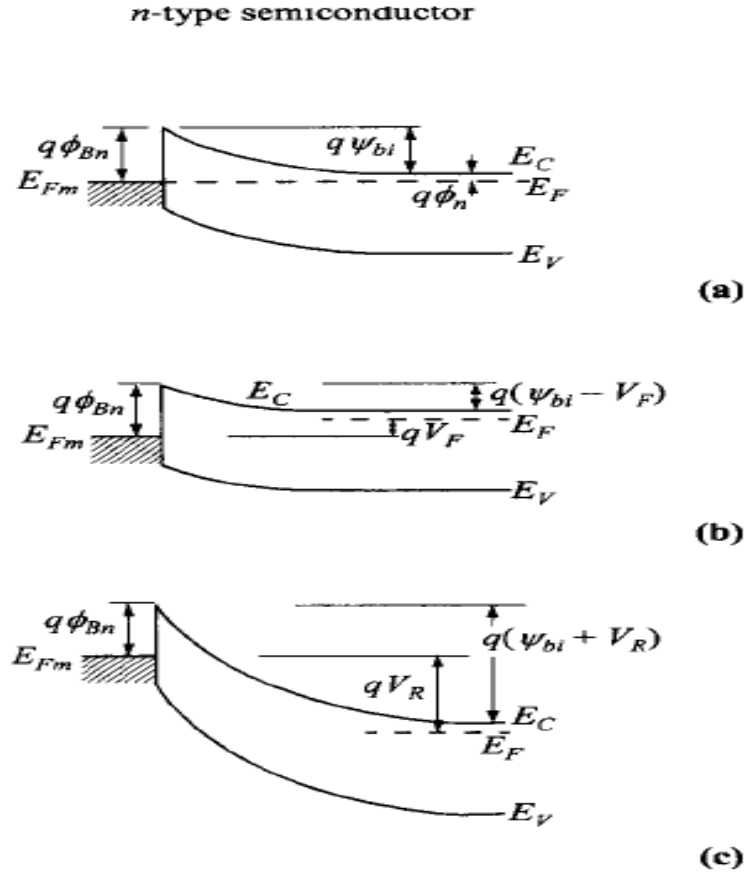


Figure 2.1: energy band diagram of metal on n-type semiconductor under different biasing conditions,(a)Thermal equilibrium,(forward bias,(c)reverse bias

where  $c_1$  is constant to be determined by boundary condition. The potential distribution can be integrated from the above equation and yields

$$v(x) = -\left(\frac{qN_D}{2\epsilon_s}\right)x^2 - c_1x + c_2 \quad (2.1.3)$$

$c_2$  is constant,The constants( $c_1$  and  $c_2$ ) can be determined by using boundary condition  $v(0) = -\phi_{Bn}$  at  $x = 0$

$$E(x) = \frac{-dv(x)}{dx} = 0 \text{ at } X = W \quad (2.1.4)$$

solving 2.1.2 and 2.1.3 in to 2.1.4 one obtains  $c_1 = \frac{-qN_D W}{\varepsilon_s}$  and  $c_2 = -\phi_{Bn}$

$$E(x) = \frac{qN_D}{\varepsilon_s}(W_D - x) \quad (2.1.5)$$

$$= E_m - \frac{qN_D x}{\varepsilon_s} \quad (2.1.6)$$

$$v(x) = (\psi_{bi} - v - \frac{kT}{q}) - \phi_{Bn} = -(\frac{qN_D}{\varepsilon_s})(\frac{x^2}{2} - Wx) - \phi_{Bn} \quad (2.1.7)$$

The potential at  $x=W$  as

$$V(W) = (\frac{qN_D W^2}{2\varepsilon_s}) - \phi_{Bn} \quad (2.1.8)$$

From the above equation the depletion width,we obtain

$$W_D = \sqrt{\frac{2\varepsilon_s(\psi_{bi} - v - \frac{kT}{q})}{qN_D}} \quad (2.1.9)$$

where the term  $\frac{kT}{q}$  arises from the contribution of the majority-carrier distribution tail (electrons in n-side) and  $\xi_m$  the maximum field strength which occurs at  $x = 0$

$$\begin{aligned} E_m = E(x=0) &= \sqrt{\frac{2qN_D}{\varepsilon_s}[\psi_{bi} - V - \frac{kT}{q}]} \\ &= \frac{2[\psi_{bi} - V - \frac{kT}{q}]}{W_D} \end{aligned} \quad (2.1.10)$$

The space charge  $Q_{sc}$ ,per unit area of the semiconductor and the depletion-layer capacitance  $C_D$  per unit area are given by

$$Q_{sc} = qN_D W_D = \sqrt{2q\varepsilon_s N_D(\psi_{bi} - V - \frac{kT}{q})} \quad (2.1.11)$$

$$C_D = \frac{\varepsilon_s}{W_D} \quad (2.1.12)$$

$$= \sqrt{\frac{q\epsilon_s N_D}{[2\psi_{bi} - V - (\frac{KT}{q})]}} \quad (2.1.13)$$

The above equation can be written in the form

$$\frac{1}{C_D^2} = \frac{2[\psi_{bi} - V - (\frac{KT}{q})]}{q\epsilon_s N_D} \quad (2.1.14)$$

$$N_D = \frac{2}{q\epsilon_s} \left[ -\frac{1}{d(\frac{1}{C_D^2})/dv} \right] \quad (2.1.15)$$

## 2.2 Image-Force Lowering

The image-force lowering, also known as the Schottky effect or Schottky-barrier lowering, is the image-force-induced lowering of the barrier energy for charge carrier emission, in the presence of an electric field. Consider a metal-vacuum system first. The minimum energy necessary for an electron to escape into vacuum from an initial energy at the Fermi level is the work function ( $q\phi_m$ ). When an electron is at a distance  $x$  from the metal, a positive charge will be induced on the metal surface. The force of attraction between the electron and the induced positive charges equivalent to the force that would exist between the electron and an equal positive Eutectic temperature charge located at  $-x$ . This positive charge is referred to as the image charge. The attractive force toward the metal, called the image force, is given by

$$F = \frac{-q^2}{4\pi\epsilon_o(2x)^2} = \frac{-q^2}{16\pi\epsilon_o x^2} \quad (2.2.1)$$

where  $\epsilon_o$ , is the permittivity of free space. The work done to an electron in the course of its transfer from infinity to the point  $x$  is given by

$$W(x) = \int F dx = \frac{-q^2}{16\pi\epsilon_o x} \quad (2.2.2)$$

This energy corresponds to the potential energy of an electron placed at a distance  $x$  from the metal surface. When an external field  $E_m$  is applied (in this example in

the-x direction), the total potential energy  $E$  as a function of distance is given by the sum.

$$\phi(x) = -\frac{q^2}{16\pi\epsilon_o x} - q|\xi|x \quad (2.2.3)$$

This equation has a maximum value. The image-force lowering  $\Delta \phi$  and the location of the lowering  $x$  are given by the condition  $\frac{d\phi(x)}{dx} = 0$

$$x_m = \sqrt{\frac{q}{16\pi\epsilon_o|\xi|}} \quad (2.2.4)$$

$$V_{max} = -e \left\{ \sqrt{\frac{eE}{4\pi\epsilon_o}} \right\} \quad (2.2.5)$$

up on substituting 2.2.4 in to 2.2.3,we get

$$\Delta \phi = \sqrt{\frac{q^3|\epsilon|}{4\pi\epsilon_o}} \quad (2.2.6)$$

Thus at high fields the Schottky barrier is considerably lowered, and the effective metal work function for thermionic emission ( $q\phi_b$ ) is reduced. These results can be applied to metal-semiconductor systems. However, the field should be replaced by the appropriate field at the interface, and the free-space permittivity  $\epsilon_0$  should be replaced by an appropriate permittivity  $\epsilon_s$ , characterizing the semiconductor medium. That is,the barrier lowering is

$$\Delta \phi = \sqrt{\frac{q^3\epsilon_m}{4\pi\epsilon_s}} \quad (2.2.7)$$

Note that inside a device such as metal-semiconductor contact, the field is not zero even without bias due to the built-in potential. Because of the larger values of  $\epsilon_s$ , in a metal-semiconductor system, the barrier lowering is smaller than that in a corresponding metal-vacuum system. For example, for  $\epsilon_s = 11.8$ ,  $\Delta\phi$  as obtained from the above equation  $1.039 \times 10^{-8}V$  for  $\epsilon = 10^5 V/cm$  and even smaller for smaller fields.

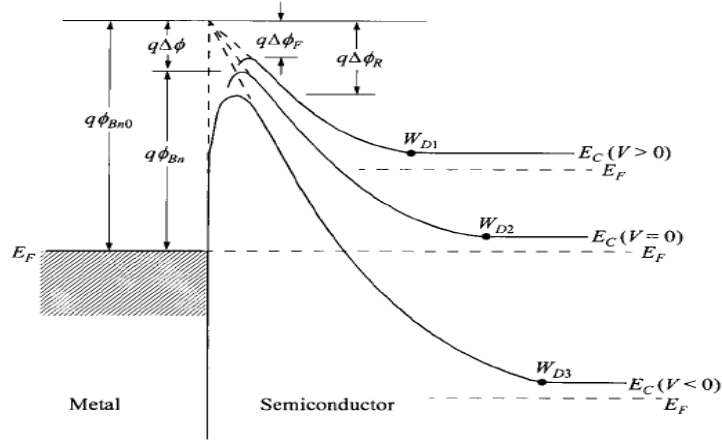


Figure 2.2: schottky effect for metal n type semiconductor under different biasing condition

Also a typical value for  $E_m$  is calculated to be less than 5nm. Although the barrier lowering is small, it does have a profound effect on current transport processes in metal-semiconductor systems. In a practical Schottky-barrier diode, the electric field is not constant with distance, and the maximum value at the surface based on the depletion approximation can be used,

$$E_m = \sqrt{\frac{2qN|\psi_s|}{\epsilon_s}} \quad (2.2.8)$$

where the surface potential  $\psi_s$  (on n-type substrate) is  $|\psi_s| = \phi_{bno} - \phi_n + V_R$ . by substitution

$$\Delta\phi = \sqrt{\frac{q\xi_m}{4\pi\epsilon_s}} = \left\{ \frac{q^3N|\psi_s|}{4\pi^2\epsilon_s^3} \right\}^{\frac{1}{4}} \quad (2.2.9)$$

Note that for forward bias ( $V > 0$ ), the field and the image force are smaller and the barrier height  $q\phi_{Bn0} - q\Delta\phi_F$  is slightly larger than the barrier height at zero bias of

$$q\phi_{Bn} = q\phi_{Bn0} - q\Delta\phi \quad (2.2.10)$$

For reverse bias ( $V_R > 0$ ), the barrier height  $q\phi_{Bn0} - q\Delta\phi_R$  is slightly smaller. In effect, the barrier height becomes bias dependent. The value  $\epsilon_s$ , may also be different from

the semiconductor static permittivity. If during the emission process, the electron transit time from the metal-semiconductor interface to the barrier maximum  $x_m$ , is shorter than the dielectric relaxation time, the semiconductor medium does not have enough time to be polarized, and smaller permittivity than the static value is expected. It will be shown, however, that for Si the appropriate permittivity's are about the same as their corresponding static values.

## 2.3 Thermionic-Emission Theory

The thermionic-emission theory by Bethe is derived from the assumptions that

- (1)The barrier height is much larger than  $kT$ ,
- (2)Thermal equilibrium is established at the plane that determines emission, and
- (3)The existence of a net current flow does not affect this equilibrium so that one can superimpose two current fluxes one from metal to semiconductor, the other from semiconductor to metal, each with a different quasi Fermi level. If thermionic emission is the limiting mechanism, then  $E_{Fn}$  is flat throughout the depletion region. Because of these assumptions, the shape of the barrier profile is immaterial and the current flow depends solely on the barrier height. The current density from the semiconductor to the metal  $J$ , is then given by the concentration of electrons with energies sufficient to overcome the potential barrier and transversing in the x-direction[6]:

$$J_{s \rightarrow m} = \int_{E_{Fn} + q\phi_B}^{\infty} qn(E)v_x(E)dE \quad (2.3.1)$$

where  $E_{Fn} + q\phi_B$ , is the minimum energy required for thermionic emission into the metal, and  $v_x$  is the carrier velocity in the direction of transport. The electron density in an incremental energy range is given by

$$n(E) = g(E) F(E) \quad (2.3.2)$$

where  $g(E)$  and  $F(E)$  are the density of states and is the probability for a taken state with energy  $E$  is occupied, respectively.

$$g(E) = \frac{8\sqrt{2}\pi}{h^3} m^{\frac{3}{2}} \sqrt{E} \quad (2.3.3)$$

and  $F(E) = \frac{1}{1+\exp(\frac{E-E_F}{KT})} \simeq \exp(-\frac{E-E_F}{KT})$  Then

$$n(E)dE = \frac{8\sqrt{2}\pi}{h^3} m^{\frac{3}{2}} \sqrt{E} \exp(-\frac{E-E_F}{KT}) \quad (2.3.4)$$

$E_c = E_F + q\phi_n$  From this  $E_F = E_c - q\phi_n$  If we postulate that all the energy of electrons in the conduction band is kinetic energy, then

$$E - E_c = \frac{1}{2} m^* \nu^2 \quad (2.3.5)$$

$$dE = m^* \nu d\nu \quad (2.3.6)$$

$$\sqrt{E - E_c} = \nu \sqrt{\frac{m^*}{2}} \quad (2.3.7)$$

Substituting in the above equation gives

$$dn \simeq 2 \left(\frac{m^*}{h}\right)^3 \exp\left\{-\frac{q\phi_n}{kT}\right\} \exp\left\{\frac{-m^* \nu^2}{2kT}\right\} (4\pi \nu^2 d\nu) \quad (2.3.8)$$

the above equation gives the number of electrons per unit volume that have velocities between  $\nu$  and  $\nu + d\nu$ , distributed over all directions. If the velocity is resolved into its components along the axes with the x-axis parallel to the transport direction, we have

$$\nu^2 = \nu_x^2 + \nu_y^2 + \nu_z^2 \quad (2.3.9)$$

With the transformation  $4\pi \nu^2 d\nu = d\nu_x d\nu_y d\nu_z$ , we obtain from the above.

$$J_{s \rightarrow m} = 2q \left(\frac{m^*}{h}\right)^3 \exp\left(-\frac{q\phi_n}{kT}\right) \int_{V_o}^{\infty} V_x \exp\left\{\frac{-m^* V_x^2}{2kT}\right\} dV_x \int_{-\infty}^{\infty} \exp\left\{\frac{-m^* V_y^2}{2kT}\right\} dV_y \int_{-\infty}^{\infty} \exp\left\{\frac{-m^* V_z^2}{2kT}\right\} dV_z \quad (2.3.10)$$

$$= \left( \frac{4\pi q m^* k^2}{h^3} \right) T^2 \exp \left\{ \frac{-q\phi_n}{kT} \right\} \exp \left\{ \frac{-m^* V_{ox}^2}{2kT} \right\} \quad (2.3.11)$$

The velocity  $v_{o_x}$  is the minimum velocity required in the x-direction to surmount the barrier and is given by Substituting in the above equation yields

$$\frac{1}{2} m^* v_{0_x}^2 = q(\psi_{b_i} - V) \quad (2.3.12)$$

Substituting in the above equation yields

$$J_{s \rightarrow m} = \left( \frac{4\pi q m^* k^2}{h^3} \right) T^2 \exp \left\{ \frac{-q\phi_{Bn}}{kT} \right\} \exp \left\{ \frac{qV}{kT} \right\} = A^* T^2 \exp \left\{ \frac{-q\phi_{Bn}}{kT} \right\} \exp \left( \frac{qV}{kT} \right) \quad (2.3.13)$$

and  $A^* = \frac{4\pi q m^* k^2}{h^3}$  is the effective Richardson constant for thermionic emission, neglecting the effects of optical-phonon scattering and quantum mechanical reflection. For free electrons ( $m^* = m_o$ ) the Richardson constant  $A = \frac{4\pi q m k^2}{h^3}$  is  $120A/cm^2 K^2$ . Note that when the image-force lowering is considered, the barrier height  $\phi_{Bn}$  is reduced by  $\Delta\phi$ .

For Si the conduction band minima occur in the  $\langle 100 \rangle$ -directions and  $m_l^* = 0.98m_o$ ,  $m_t^* = 0.19 m_o$ . The minimum value of  $A^*$  occurs for the  $\langle 100 \rangle$ -directions:

$$\left( \frac{A^*}{A} \right)_{n-si\langle 100 \rangle} = \frac{2m_t^*}{m_o} + \frac{4\sqrt{m_l^* m_t^*}}{m_o} = 2.1 \quad (2.3.14)$$

In the  $\langle 111 \rangle$ -directions all minima contribute equally to the current, yielding the maximum  $A^*$ :

$$\left( \frac{A^*}{A} \right)_{n-si\langle 111 \rangle} = \frac{6}{m_o} \sqrt{\frac{(m_t^*)^2 + 2m_l^* m_t^*}{3}} = 2.2 \quad (2.3.15)$$

For holes in Si and GaAs the two energy maxima at  $k = 0$  give rise to approximately isotropic current flow from both the light and heavy holes. Adding the currents due to these carriers, we obtain

$$\left\{ \frac{A^*}{A} \right\}_{p-typ} = \frac{m_{lh}^* + m_{hh}^*}{m_o} \quad (2.3.16)$$

Since the barrier height for electrons moving from the metal into the semiconductor remains the same under bias, the current flowing into the semiconductor is thus unaffected by the applied voltage. It must therefore be equal to the current flowing from the semiconductor into the metal when thermal equilibrium prevails (i.e., when  $V = 0$ ). This corresponding current density is obtained from Eq. 2.1.12 by setting  $v = 0$

$$J_{m \rightarrow s} = -A^*T^2 \exp \left\{ \frac{-q\phi_{Bn}}{kT} \right\} \quad (2.3.17)$$

Then the total current density is given by  $J_n = J_{s \rightarrow m} - J_{m \rightarrow s}$

$$J_n = [A^*T^2 \exp \left\{ \frac{-q\phi_{Bn}}{kT} \right\}] [\exp \left( \frac{qV}{kT} \right) - 1] \quad (2.3.18)$$

$$= J_{TE} \left\{ \exp \left( \frac{qV}{kT} \right) - 1 \right\} \quad (2.3.19)$$

where,

$$J_{TE} = A^*T^2 \exp \left\{ \frac{-q\phi_{Bn}}{kT} \right\} \quad (2.3.20)$$

The above equation is similar to the transport equation for p-n junctions. However, the expressions for the saturation current densities are quite different. An alternative approach to derive the thermionic-emission current is the following. Without decomposing the velocity components, only electrons with energy above the barrier will contribute to the forward current. This number of electrons above the barrier is given by

$$n = N_c \exp \left\{ \frac{-q(\phi_{Bn} - V)}{kT} \right\} \quad (2.3.21)$$

$$N_c = \frac{1}{4} \left\{ \frac{2m^*K_B T}{\pi \hbar^2} \right\}^{\frac{3}{2}} \quad (2.3.22)$$

It is known that for a Maxwellian distribution of velocities, the current from random motion of carriers across a plane is given by

$$J = nq \frac{v_{ave}}{4} \quad (2.3.23)$$

where  $v_{ave}$  is the average thermal velocity,

$$v_{ave} = \sqrt{\frac{8kT}{\pi m^*}} \quad (2.3.24)$$

Substitution of Eqs. 2.3.20 and 2.3.22 into Eq.2.3.21 gives

$$J = \frac{4(kT^2)q\pi m^*}{h^3} \exp \left\{ \frac{-q(\phi_{Bn} - V)}{kT} \right\} \quad (2.3.25)$$

## 2.4 Diffusion Theory

The diffusion theory by Schottky is derived from the assumptions that

1. the barrier height is much larger than  $kT$ ,
2. the effect of electron collisions within the depletion region, i.e. diffusion, is included,
3. the carrier concentrations at  $x = 0$  and  $x = W_D$ , are unaffected by the current flow (i.e., they have their equilibrium values), and
4. the impurity concentration of the semiconductor is non degenerate.

When an n-type semiconductor is connected to a metal of a sufficiently high work function, electrons from the semiconductor leak out into the adjacent metals. The electron density at the interface between the metal electrode and the semiconductor is reduced below its equilibrium bulk value  $n_{i0}$ , and thereby a positive space-charge region is created within the semiconductor near the metal contact. The corresponding negative

charge, to render the total device neutral is located at the metal/semiconductor interface. The space-charge layer in the semiconductor results in a field ramp and a potential step, referred to as the Schottky barrier. The electron density at the metal/semiconductor interface is given by[4]

$$n_c = n(x = 0) = N_c \exp\left(-\frac{e\phi_{ms}}{kT}\right) \quad (2.4.1)$$

Where  $N_c$  is the effective level density at the metalsemiconductor interface. This interface electron density  $n_c$  is initially assumed to be independent of current and applied voltage:  $n_c = n_j(x = o^+, j \neq 0)$

where  $n_j$  is the electron density at the semiconductor side of the interface which will later be allowed to change as a function of the current. The electron density in the bulk is given by the density of the shallow, uncompensated donors  $n_{10} \approx N_d$ . The space charge density

$$\rho(x) = e[p_d - n(x)] \approx e[N_d - n(x)] \approx eN_d \quad (2.4.2)$$

for  $0 \leq x < x \leq D'$  independent of  $n$  in a substantial fraction of this junction-region (*with*  $x'_D < x_D$ ) .  $p_d$  is the density of positively charged, ionized donors. In using this constant space charge within the entire width of the Schottky barrier (i.e., assuming  $x'_D = x_D \simeq 810^{-6}cm$ ), the resulting Schottky approximation permits a major simplification of the governing set of equations[4]

$$\frac{dn}{dx} = \frac{J_n - e\mu_n n F}{\mu_n kT} \quad (2.4.3)$$

$$\frac{dF}{dx} = \frac{eN_d}{\epsilon_{st}\epsilon_o} \quad (2.4.4)$$

$$\frac{d\psi_n}{dx} = F \quad (2.4.5)$$

This allows decoupling of the Poisson equation from the transport equation. Integration of (2.4.4) yields

$$F(x) = F_c + \frac{eN_d}{\epsilon_{st}\epsilon_o} x \quad (2.4.6)$$

that is, the field decreases linearly with increasing distance from the metal/ semiconductor interface, with  $F_c$ , the maximum value of the field at  $x = 0$ , used here as the integration constant. From the integration of (2.4.4) after insertion of (2.4.6), one obtains the electrostatic electron potential

$$\psi_n(x) = \psi_{n,D} + F_c x + \frac{eN_d}{2\epsilon_{st}\epsilon_o} x^2 \quad (2.4.7)$$

which decreases parabolically with increasing  $x$ . As integration constant, we used the electron diffusion potential  $\psi_{n,D}$  which is appropriate for zero current. Then, the diffusion potential can also be approximated by the product of maximum barrier field and barrier width.

$$\psi_{n,D} = -\frac{F_c x_D}{2} \quad (2.4.8)$$

For the barrier field at  $x = x_D$  one obtains

$$F_c = -\frac{eN_d x_D}{\epsilon_{st}\epsilon_o} \quad (2.4.9)$$

After combining the above equation and eliminating  $x_D$ , one can express the barrier field at zero current as a function

$$F_c = -\sqrt{\frac{2eN_d\psi_{n,D}}{\epsilon_{st}\epsilon_o}} \quad (2.4.10)$$

When inserting  $F_c$ (barrier field) at zero current as a function of  $\psi_{n,D}$  yields

$$\psi(x) = \frac{1}{\sqrt{2}} \frac{kT}{e} \left[ \sqrt{\frac{2e\psi_{n,D}}{KT}} - \frac{x}{L_D} \right]^2 \quad (2.4.11)$$

$L_D$  is the Debye length, which is a characteristic length for changing  $\psi_n(x)$  and  $F(x)$ .

$$L_D = \sqrt{\frac{\epsilon_{st}\epsilon_o kT}{e^2 N_d}} \quad (2.4.12)$$

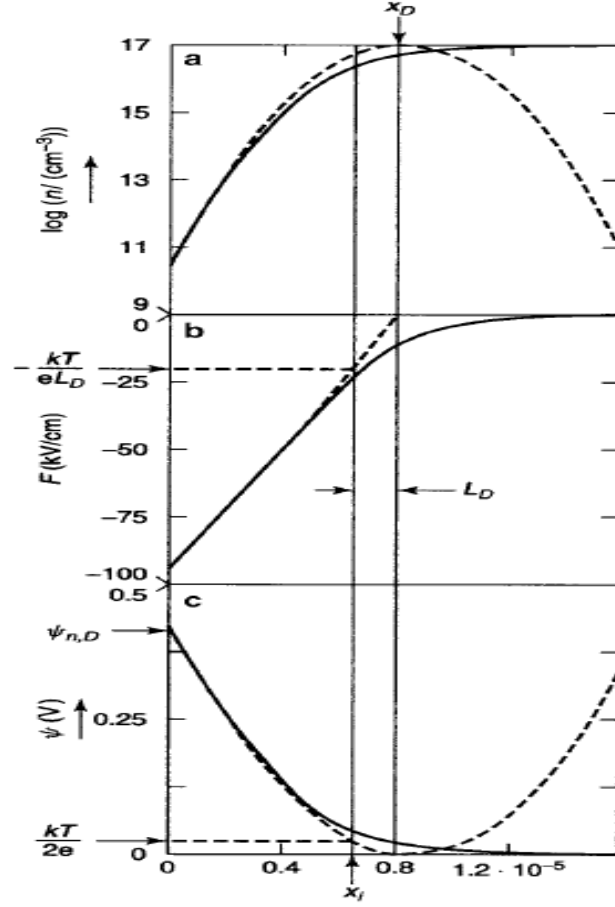


Figure 2.3: The solid curves shows the exact solution of (2.4.3-2.4.5) and the dashed curves the Schottky approximations (2.4.6-2.4.7)

The barrier layer thickness can be expressed in terms of  $L_D$  by combining the above equation by eliminating  $F_c$  yields

$$x_D = L_D \sqrt{\frac{2e\psi_{n,D}}{kT}} \quad (2.4.13)$$

which means that  $x_D$  is usually a few (typically 3-6) Debye lengths thick, since  $\psi_{n,D}$  is typically on the order of  $10kT/e$ . The electron density distribution can be obtained for  $j_n = 0$  from the transport equation  $\frac{dn}{dx} = -\frac{e}{kT}nF(x)$ . After replacing  $F(x)$  by  $\frac{d\psi_n(x)}{dx}$  one obtains the Boltzmann distribution by integration  $n(x) = n_{10} \exp(-\frac{e\psi_n(x)}{kT})$ .

When inserting  $F(x)$  using as a convenient parameter

$$\frac{1}{L^2 D} = \frac{e}{kT} \frac{e N_d}{\epsilon_{st} \epsilon_o} \quad (2.4.14)$$

$$n(x) = n_{10} \exp\left[\left(\frac{e\psi_{n,D}}{kT} + \frac{eF_c(x)}{kT} + \frac{x^2}{2L^2 D}\right)\right] \quad (2.4.15)$$

The electron potential step between bulk and metal/semiconductor interface is obtained by setting  $x = 0$ , yielding the diffusion potential for zero current with  $n(x = 0) = n_c$ :

$$\psi_{n,D} = \frac{kT}{e} \ln\left(\frac{n_c}{n_{10}}\right) \quad (2.4.16)$$

This electron diffusion potential depends only on the ratio of the bulk and interface densities of carriers.

The Debye length is also the position (counting from  $x = x_D$ ) at which  $n(x)$  for zero current has its maximum slope, the opposing diffusion and drift currents have their maximum value, as one obtains from differentiation of (3.11)

$$\frac{d^2 n}{dx^2} = -\frac{e}{kT} \left( \frac{ndF}{dx} + \frac{Fdn}{dx} \right) = 0 \quad (2.4.17)$$

which yields for the inflection point of  $n(x)$ , located at  $x = x_i$

$$F(x_i) = F_c \sqrt{\frac{kT}{2e\psi_D}} = -\sqrt{\frac{kTN_d}{\epsilon_{st}\epsilon_o}} = -\frac{kT}{eL_D} \quad (2.4.18)$$

when compared with the value obtained from the Poisson equation:

$$F(x_i) = \frac{eN_d(x_D - x_i)}{\epsilon_{st}\epsilon_o} \quad (2.4.19)$$

yields  $x_i = x_D - L_D$ . When introducing the Schottky approximation for  $F(x)$  into the transport equation, one obtains a linear differential equation for  $n(x)$

$$\frac{dn}{dx} + \frac{e}{kT} \left( F_c + \frac{eN_d}{\epsilon_{st}\epsilon_o x} \right) n(x) - \frac{j_n}{\mu_n kT} = 0 \quad (2.4.20)$$

integrating the above equation yields the general solution where  $J_n = \text{constant}$

$$n(x') = n_c \exp\left(-\frac{e[\psi_n(x') - \psi_{n,D}]}{kT}\right) + \frac{j_n}{e\mu_n F_c} \cdot 2 \left\{ \sqrt{\frac{e\psi_{n,D}}{kT}} \cdot D\left(\sqrt{\frac{e\psi_n}{kT}}\right) \right\} \quad (2.4.21)$$

where  $D(\xi)$  is Dawsons integral:

$$D(\xi) = \exp(-\xi^2) \int_0^\xi \exp(t^2) dt \quad (2.4.22)$$

For  $\xi > 2$ , Dawsons integral can be approximated by  $D(\xi) = (\frac{1}{2\xi})(1 + \frac{1}{2\xi^2} + \frac{3}{4\xi^4} + \dots)$  the first term of which is sufficiently accurate for  $\xi > 4$ , yielding

$$D(\xi) \approx \frac{1}{2\xi} \quad (2.4.23)$$

Using only the first term of the Dawsons integral approximation, one can reduced (2.4.20) to a simple expression

$$n(x') = n_c \exp\left\{-\frac{e[\psi_n(x') - \psi_{n,D}]}{kT}\right\} + \frac{j_n}{e\mu_n F(x')} \quad (2.4.24)$$

$f(x') = \sqrt{\frac{2eN_d\psi_n(x')}{\epsilon_{st}\epsilon_o}}$ , One obtains an analytical expression of the current voltage characteristic when solving (2.4.23) for  $j_n$  and using the boundary condition  $n(x = 0) = n_c$ . This yields

$$j_n = e\mu_n n_c F_j \left\{ \exp\left[-\frac{e(\psi_{n,j} - \psi_{n,D})}{KT}\right] - 1 \right\} \quad (2.4.25)$$

with

$$F_j = F(x = 0) = \sqrt{\frac{2eN_d\psi_{n,j}}{\epsilon_{st}\epsilon_o}} \quad (2.4.26)$$

$$\psi_{n,j} = \psi_n(x = 0) \quad (2.4.27)$$

The index  $j$  identifies the value of the variable at the interface for a given current  $j_n$ . This (2.4.24) is the diode equation for which the expression  $[\exp() - 1]$  is typical. The applied voltage, defined as

$$V = -\frac{1}{e} [E_F(x = 0) - E_F(x = d_1)] \quad (2.4.28)$$

can be easily obtained in the range where  $E_c(x)$  and  $E_F(x)$  run parallel to each other which yields

$$V = \psi_{n,j} - \psi_{n,D} \quad (2.4.29)$$

As an approximation, the often used classical diode equation of drift-current-limited Schottky barriers.

$$j_n = e\mu_n n_c F_j \left[ \exp\left(\frac{eV}{kT}\right) - 1 \right] \quad (2.4.30)$$

and with the field at the barrier interface given by

$$F_j = \sqrt{\frac{2eNd(\psi_{n,D} - V)}{\epsilon_{st}\epsilon_o}} \quad (2.4.31)$$

The modified schottky potential barrier at the metal/semiconductor boundary prevents the leaking-out of metal electrons into the semiconductor. The maximum diffusion current that can be drawn from this metal surface is given by the Richardson-Dushman emission[4].

$$j_n = en_c v_n^* \quad (2.4.32)$$

with  $v_n^* = \frac{v_n}{\sqrt{6\pi}}$  and  $v_n$  as the rms velocity of electrons  $v_n = \sqrt{\frac{3kT}{m_n}}$  With a bias, the current at  $x = \delta^+$  can be described as the difference of two components, one which passes through this interface from left to right ( $\vec{j}_n$ ) and one which passes from right to left ( $\overleftarrow{j}_n$ )

$$j_n = (\vec{j}_n) - (\overleftarrow{j}_n) \quad (2.4.33)$$

When assuming each of these currents to be Richardson-Dushman currents at  $x = \delta^+$ , with

$$(\vec{j}_n) = en_c v_n^* \text{ and } (\overleftarrow{j}_n) = en_j v_n^* \quad (2.4.34)$$

The jump of the carrier density at the interface, between the metal and the semiconductor is essential to be recognized for any discussion of such electrical contact. In recognizing this we obtain for the net current through the interface

$$j_n = ev_n^*(n_j - n_c) \quad (2.4.35)$$

With the modified boundary condition the above equation, we can now calculate the current.voltage characteristics from (3.33) and, replacing  $n(x = \delta^+)$  with  $n_j$  from (3.46); this yields

$$j_n = \frac{ev_n^*n_c \exp\left[\frac{e(\psi_n, D - \psi_n, j)}{kT}\right] - 1}{1 - \frac{v_n^*}{\mu_n j}} \quad (2.4.36)$$

The replacement of  $\psi_n, D - \psi_n, j$ , yielding again (3.39) which leads to the modified Schottky diode equation

$$j_n = \frac{ev_n^*n_c \exp\left[\frac{ev}{kT}\right] - 1}{1 + \frac{v_n^*}{\mu_n j}} \quad (2.4.37)$$

For low fields ( $|\mu_n \ll v_n^*|$ ) in forward and low reverse bias, this equation reverts back to the drift-limited Schottky diode equation

$$j_n = en_c \mu_n F_j \exp\left[\frac{ev}{kT}\right] - 1 \quad (2.4.38)$$

For high fields ( $\mu_n F_j \gg v_n^*$ ), i.e., for sufficiently high reverse bias, the diffusion-limited Schottky diode equation

$$j_n = en_c v_n^* \exp\left[\frac{ev}{kT}\right] - 1 \quad (2.4.39)$$

## 2.5 Thermionic-Emission-Diffusion Theory

A synthesis of the thermionic-emission and diffusion approaches described above has been proposed by Crowell and Sze[6]. This approach is derived from the boundary condition of a thermionic recombination velocity  $v_R$  near the metal-semiconductor

interface. Since the diffusion of carriers is strongly affected by the potential configuration in the region through which the diffusion occurs, we consider the electron potential energy [or  $E_c(x)$ ] versus distance incorporating the Schottky lowering effect. We consider the case where the barrier height is large enough that the charge density between the metal surface and  $x = W_D$  is essentially that of the ionized donors (i.e., depletion approximation). The applied voltage ( $V$ ) between the metal and the semiconductor bulk would give rise to a flow of electrons toward the metal. Throughout the region between  $x_m$  and  $W_D$ , where the electron

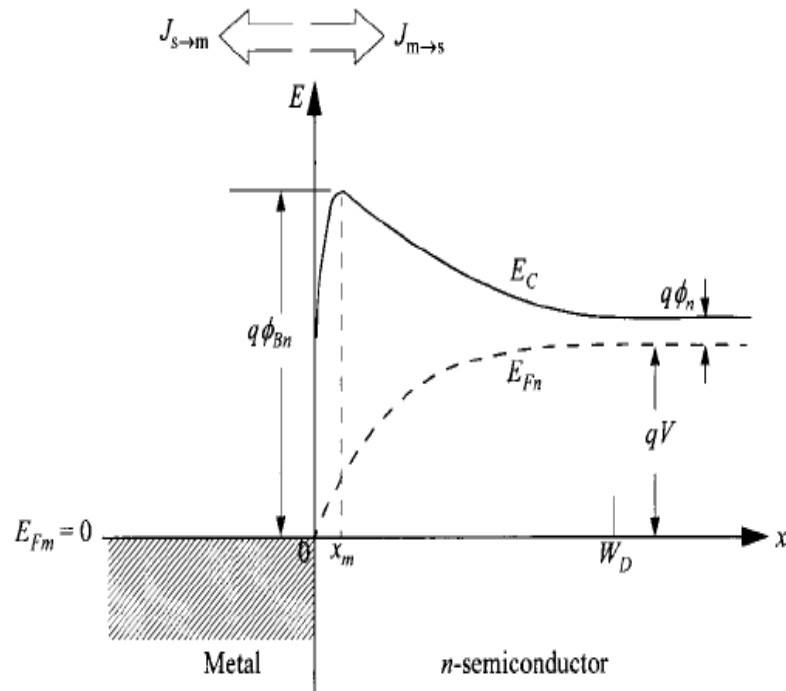


Figure 2.4: energy band diagram incorporating the schottky effect to show the derivation of thermionic-emission diffusion theory and tunneling current

$$J = n \mu_n \frac{dE_{Fn}}{dx} \quad (2.5.1)$$

density at any point  $x$  is given by

$$n = N_c \exp\left(\frac{-(E_c - E_{Fn})}{kT}\right) \quad (2.5.2)$$

We will assume that the region between  $x_m$ , and  $W_D$  is isothermal and that the electron temperature  $T$  is equal to the lattice temperature. If the portion of the barrier between  $x_m$  and the interface ( $x = 0$ ) acts as a sink for electrons, we can describe the current flow in terms of an effective recombination velocity  $v_R$  at the potential energy maximum  $x_m$ :

$$J = q(n_m - n_o)V_R \quad (2.5.3)$$

where  $n_m$ , is the electron density at  $x_m$ , when the current is flowing

$$n_m = N_c \exp\left\{\frac{E_{Fn}(x_m) - E_c(x_m)}{kT}\right\} \quad (2.5.4)$$

$$= N_c \exp\left\{\frac{E_{Fn}(x_m) - q \phi_{Bn}}{kT}\right\} \quad (2.5.5)$$

$n_o$  is a quasi-equilibrium electron density at  $x_m$  the density that would occur if it were possible to reach equilibrium without altering the magnitude or position of the potential energy maximum, i.e.,  $E_{Fn}(x_m) = E_{Fm}$

$$n_o = N_c \exp\left(-\frac{q \phi_{Bn}}{kT}\right) \quad (2.5.6)$$

Another boundary condition, taking  $E_{Fm} = 0$  as reference, is

$$E_{Fm}(W_D) = qV \quad (2.5.7)$$

If  $n$  is eliminated from Eqs. 2.5.1 and 2.5.2 and the resulting expression for  $E_{Fn}$  is integrated between  $x_m$  and  $W_D$ , Then

$$\exp\left\{\frac{E_{Fn}(x_m)}{kT} - \exp\left(\frac{qV}{kT}\right)\right\} = \frac{-J}{\mu_n N_c kT} \int \exp\left(\frac{E_c}{kT}\right) dx \quad (2.5.8)$$

using equation 2.5.3 in to 2.5.8 and integrating we set

$$\exp\left\{\frac{E_{Fn}(x_m)}{kT}\right\} = \frac{V_D \exp\left(\frac{qV}{kT}\right) + V_R}{V_D + V_R} \quad (2.5.9)$$

Where

$$v_D = D_n \exp\left(\frac{q\phi_{Bn}}{kT}\right) \int_{x_m}^{W_D} \exp\left(\frac{E_c}{kT}\right) dx \quad (2.5.10)$$

is an effective diffusion velocity associated with the transport of electrons from the edge of the depletion layer  $W_D$ , to the potential energy maximum  $x_m$ . Substituting Eq. 2.5.9 into Eq. 2.5.3 gives the end result of the thermionic-emission-diffusion theory

$$J_{TED} = \frac{q N_c v_R}{1 + (v_R/v_D)} \exp\left\{-\frac{q \phi_{Bn}}{kT}\right\} \left\{\exp\left(\frac{qV}{kT}\right) - 1\right\} \quad (2.5.11)$$

In this equation, the relative values of  $v_R$  and  $v_D$  determines the relative contribution of thermionic emission versus diffusion. The parameter  $v_D$  can be evaluated as the Dawsons integral and can be approximated by  $v_D \approx \mu_n \varepsilon_m$  in this case of depletion region. If the electron distribution is Maxwellian for  $x \geq x_m$  and if no electrons return from the metal other than those associated with the current density  $q n_o v_R$  the semiconductor acts as a thermionic emitter. Then  $v_R$  is the thermal velocity given by

$$v_R = \int_0^{W_D} v_x \exp\left(\frac{-m^* v_x^2}{2kT}\right) dv_x / \int_{-\infty}^{\infty} \exp\left\{\frac{-m^* v_x^2}{2kT}\right\} dv_x \quad (2.5.12)$$

$$= \sqrt{\frac{kT}{2m^* \pi}} = \frac{A^* T^2}{q N_c} \quad (2.5.13)$$

where  $A^*$  is the effective Richardson constant. At 300 K,  $v_R$  is  $5.2 \times 10^6$  cm/s for  $\langle 111 \rangle$  n-type Si. It can be seen that if  $V_D \gg V_R$  the pre-exponential term in equation 2.5.11 is dominated by  $v_R$  and the thermionic-emission theory applies ( $J_{TED} = J_{TE}$ ).

If, however,  $v_D \ll v_R$ , the diffusion process is the limiting factor ( $J_{TED} = J_D$ ).

In summary, Eq. 2.5.11 gives a result that is a synthesis of Schottky's diffusion theory and Bethes thermionic-emission theory, and it predicts currents in essential agreement with the thermionic-emission theory if  $\mu \varepsilon(x_m) > v_R$ . The latter criterion is more rigorous than Bethes condition  $\varepsilon(x_m) > kT/q \lambda$ , where  $\lambda$  is the carrier mean free path.

In the preceding section a recombination velocity  $v_R$  associated with thermionic emission was introduced as a boundary condition to describe the collecting action of the metal in a Schottky barrier. In many cases an appreciable probability exists that an electron which crosses the potential energy maximum will be back-scattered by electron optical-phonon scattering. As a first approximation the probability of electron emission over the potential maximum can be given by  $f_p = \exp(-x_m/\lambda)$ . In addition, the electron energy distribution can be further distorted from a Maxwellian distribution because of quantum-mechanical reflection of electrons by the Schottky barrier, and also because of tunneling of electrons through the barrier. The ratio of the total current flow, considering the quantum-mechanical tunneling and reflection, to the current flow neglecting these effects depends strongly on the electric field and the electron energy measured from the potential maximum.

The complete expression of the J-V characteristics taking into account  $f_p$  and  $f_Q$  is thus

$$J = A^{**} T^2 \exp\left(\frac{-q \phi_{Bn}}{kT}\right) \left[ \exp\left(\frac{qV}{kT}\right) - 1 \right] \quad (2.5.14)$$

where,

$$A^{**} = \frac{f_p f_Q A^*}{1 + (f_p f_Q v_R / v_D)}$$

The impacts of these effects are reflected in the reduced effective Richardson constant from  $A^*$  to  $A^{**}$ , by as much as 50 percent.

Figure 2.5 shows the calculated room-temperature values of  $A^{**}$  for metal-systems with an impurity concentration of  $10^{16} \text{ cm}^{-3}$ . We note that for electrons (n-type Si),

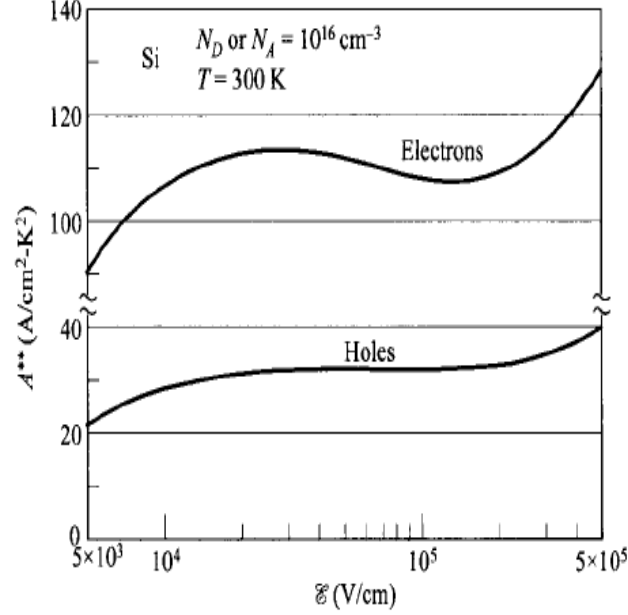


Figure 2.5: calculated effective Richardson constant  $A^{**}$  versus electric field for metal-silicon barriers

$A^{**}$  in the field range  $10^4$  to  $2 \times 10^5 V/cm^2 K^2$  remains essentially at a constant value of about  $110 A/cm^2 k^2$ . For holes (p-type Si),  $A^{**}$  in this field range also remains essentially constant but at a considerably lower value ( $\approx 30 A/cm^2 K^2$ ). For n-type GaAs,  $A^{**}$  has been calculated to be  $4.4 A/cm^2 - K^2$

We conclude from the foregoing discussions that at room temperature in the electric field range of  $10^4$  to about  $10^5 V/cm$ , the current transport mechanism in most Si and GaAs Schottky-barrier diodes is mainly due to thermionic emission of majority carriers. The spatial dependence of the electron Fermi level  $E_{Fn}$  near the metal-semiconductor interface has been studied by substituting Eqs. 2.1.2 and 2.5.2 into Eq. 2.5.1 and evaluating the difference,  $E_{Fn}(W_D) - E_{Fn}(0)$ . The  $E_{Fn}$  is essentially flat throughout the depletion region. The difference  $E_{Fn}(W_D) - E_{Fn}(0)$  for a Au-Si diode with  $N_D = 1.2 \times 10^{15} cm^{-3}$  is the only  $8 meV$  for a forward bias of 0.2 V at

300K. At higher doping levels the difference is even smaller. These results further confirm that for high-mobility semiconductors with moderate doping, the thermionic-emission theory is applicable.

## 2.6 TUNNELING CURRENT

While tunneling electrons from a metal originate from the Fermi level. In semiconductors the density of state function shows a gap near  $E_F$  and has permitted ranges at the valence and conduction bands. In addition, there are surface states that can be occupied and become a significant source of tunneling electrons. The necessary filling (or replenishing) of these states is a function of the relative position of the Fermi level which, in turn, is determined by the band bending near the surface, as indicated in the previous section.

Tunneling break down occurs in heavily doped p-n junction in which the Depletion region width  $W$  is about 10nm. The tunneling current obtained by using Wentzel Kramers Brilloin (WKB) approximation[11].

The WKB approximation states that since in a constant potential, the wavefunction solutions of the Schrodinger equation are of the form of simple plane waves, then

$$k = \frac{2\pi}{\lambda} = \sqrt{\frac{2m(E - U)}{\hbar^2}} \quad (2.6.1)$$

Now, if the potential  $U = U(x)$  changes slowly with  $\chi$ , the solution of schrodinger equation can also be written of the general form  $\psi(x) = Ae^{i\phi(x)}$ , where  $\phi(x) = \chi k(x)$

For constant potential case,  $\psi(x) = \pm kx$  so the phase changes linearly with  $\chi$

In a slowly varying potential  $\phi(x)$  should vary slowly from the linear case  $\pm k\chi$

$$k(x) = \sqrt{\frac{2m(E - U(x))}{\hbar^2}}, E > U(x) \quad (2.6.2)$$

$$k(x) = -i\sqrt{\frac{2m(U(x) - E)}{\hbar^2}} = -ik(x), U(x) > E \quad (2.6.3)$$

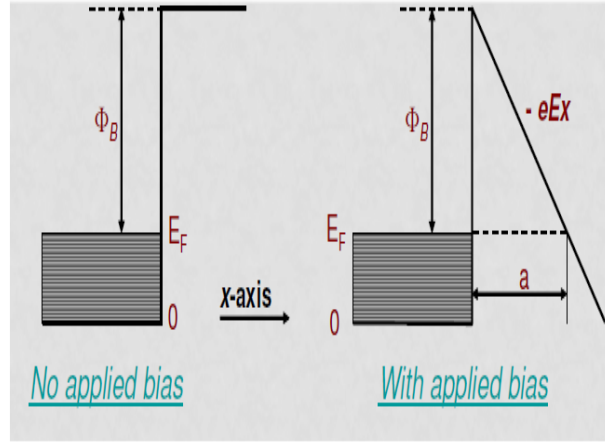


Figure 2.6: energy diagram

The difference between Fermi level and the top of barrier is denoted by  $\phi_B$   
 According to WKB approximation, the tunneling coefficient is  $T(x) \sim \exp[-2 \int_0^a \gamma(x) dx]$   
 Where  $\gamma$  is defined by[11]

$$\gamma(x) = \sqrt{\frac{2m^*}{\hbar^2}(\phi_B - eEx)} \quad (2.6.4)$$

With applied bias,  $V(z) = E_G(1 - \frac{z}{W})$  the transmission coefficient

$$T = e^{-2\alpha} \quad (2.6.5)$$

The attenuation the barrier is thus

$$\begin{aligned} 2\alpha &= 2 \int_0^{z_0} \sqrt{\frac{2m}{\hbar^2} [V(z) - E(z)]} dz \\ &= 2 \int_0^{z_0} \sqrt{\frac{2m}{\hbar^2} [E_G(1 - \frac{z}{W}) - E_Z]} dz \\ &= 2 \int_0^{z_0} \sqrt{\frac{2m E_G}{\hbar^2} [1 - \frac{z}{W} - \frac{E_Z}{E_G}]} dz \\ &= 2 \int_0^{z_0} \sqrt{\frac{2m E_G}{\hbar^2}} \sqrt{1 - \frac{z}{W} - \frac{E_Z}{E_G}} dz (\frac{-z}{W}) (-W) \\ &= 2 \int_0^{z_0} \sqrt{\frac{2m E_G}{\hbar^2}} \sqrt{1 - \frac{z}{W} - \frac{E_Z}{E_G}} dz (\frac{-z}{W}) \end{aligned}$$

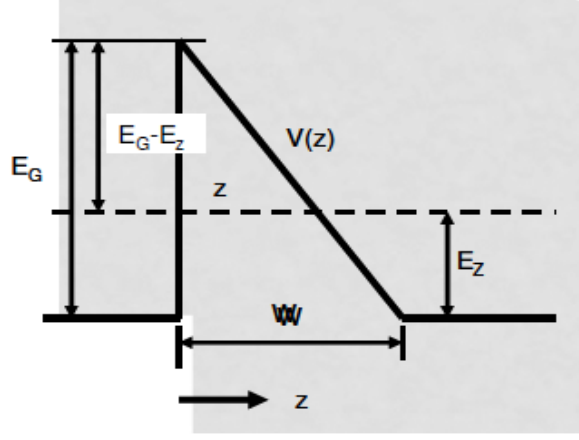


Figure 2.7: tunneling probability

$$= (-2W) \sqrt{\frac{2mE_G}{\hbar^2}} \left(1 - \frac{z}{W} - \frac{E_Z}{E_G}\right)^{\frac{3}{2}} \Big|_0^{z_0}$$

$$2\alpha = -\frac{4W}{3} \sqrt{\frac{2mE_G}{\hbar^2}} \left[ \left(1 - \frac{z}{W} - \frac{E_Z}{E_G}\right)^{\frac{3}{2}} - \left(1 - \frac{E_Z}{E_G}\right)^{\frac{3}{2}} \right] \quad (2.6.6)$$

where,  $1 - \frac{z}{W} - \frac{E_Z}{E_G} = 1 - \frac{Eg - Ez}{Eg} - \frac{Ez}{Eg} = \frac{Eg - Ez}{Eg} - \frac{Eg - Ez}{Eg}$

Hence,

$$\alpha = \frac{4W}{3} \sqrt{\frac{2mE_G}{\hbar^2}} \left(1 - \frac{E_Z}{E_G}\right)^{\frac{3}{2}} \approx \frac{4W}{3} \sqrt{\frac{2mE_G}{\hbar^2}} \left(1 - \frac{3E_Z}{2E_G}\right) \quad (2.6.7)$$

And

$$T(EZ) = e^{-2\alpha} = e^{-\frac{4W}{3} \sqrt{\frac{2mE_G}{\hbar^2}}} e^{\frac{2W}{Eg} \sqrt{\frac{2mE_G}{\hbar^2}} EG} = T_o e^{\frac{E_Z}{E_o}} \quad (2.6.8)$$

where,  $E_o = \frac{Eg}{2W} \sqrt{\frac{\hbar^2}{2mEg}} = \sqrt{\frac{\hbar^2 Eg^2}{2mEg}} \frac{1}{2W} = \frac{1}{2W} \sqrt{\frac{\hbar^2 Eg}{2m}}$

The final expression for the Fowler-Nordheim tunneling coefficient is:

$$T \propto \exp\left[-\frac{4\sqrt{2m} \phi_B^{\frac{3}{2}}}{3eE\hbar}\right] \quad (2.6.9)$$

The net tunneling current from metal to semiconductor can be written as the net difference between current flowing from metal to semiconductor and vice versa.

$$J = J_{m \rightarrow s} - J_{s \rightarrow m}$$

The current density through the two interfaces depends on the perpendicular component of the wave vector  $k_x$ , the transmission coefficient  $T_c$ , the perpendicular velocity  $v_x$ , the density of states  $g_c$  and the distribution function at both sides of the barrier:

$$dJ_{m \rightarrow s} = qT_c(k_x)V_x g_m(k_x)f_m(E)[1 - f_m(E)]dk_x \quad (2.6.10)$$

$$dJ_{s \rightarrow m} = qT_c(k_x)V_x g_s(k_x)f_s(E)[1 - f_s(E)]dk_x \quad (2.6.11)$$

Considering the quantized wave vector components within a cube of side L yields for the density of states within the cube:

$$g(k_x, k_y, k_z) = \frac{L^3}{(2\pi)^3} \cdot \frac{1}{\Delta k_x \Delta k_y \Delta k_z} = \frac{1}{4\pi^3}, \Delta k_i = \frac{2\pi}{L} (\Delta n_i) \quad (2.6.12)$$

where  $g = \frac{4}{4\pi^3}$  [with spin degeneracy]

$$v_x = \frac{1}{\hbar} \cdot \frac{\partial E}{\partial K_x} = \frac{\hbar k_x}{m_{eff}} \cdot V_x dk_x = \frac{1}{\hbar} \cdot dE_x \quad (2.6.13)$$

Hence, the current density becomes  $dJ_{m \rightarrow s} = \frac{q}{4\pi^3 \hbar} T(E_x) dE_x \int \int f_m(E)[1 - f_s(E)] dk_y dk_z$   
 $dJ_{s \rightarrow m} = \frac{q}{4\pi^3 \hbar} T_c(k_x) dE_x \int \int f_2(E)[1 - f_m(E)] dk_y dk_z$  using polar coordinates for the parallel wave vector components  $k_\rho = \sqrt{k_y^2 + k_z^2}$

$$J_{m \rightarrow s} = \frac{4\pi m_{eff} q}{\hbar} \cdot \int T_c(E_x) dE_x \int f_1(E)[1 - f_s(E)] dE_\rho \quad (2.6.14)$$

$$J_{s \rightarrow m} = \frac{4\pi m_{eff} q}{\hbar} \cdot \int T_c(E_x) dE_x \int f_2(E)[1 - f_m(E)] dE_\rho \quad (2.6.15)$$

The total energy is sum of longitudinal part  $E_x$  and transverse part  $E_\rho$  Evaluating the difference, the net current through the interface equals:  $J = J_{m \rightarrow s} - J_{s \rightarrow m}$

$= \frac{4\pi m_{eff} q}{\hbar^3} \int_{E_{min}}^{E_{max}} T_c(E_x) dE_x \int_0^\infty [f_1(E) - f_2(E)] dE_\rho$  This expression is usually written

as an integral over the product of two independent parts which only depend upon the energy perpendicular to the interface. The transmission coefficient  $T_c(\text{Ex})$  and the supply function  $N(\text{Ex})$

$$J = \frac{4\pi m_{eff} q}{\hbar^3} \int T_c(E_x) N(E_x) dE(x) \quad (2.6.16)$$

The above expression is known as the Tsu- Esaki formula. The supply function describes the difference in the supply of carriers at the interfaces.

$$N(E_x) = \int_0^\infty [f_1(E) - f_2(E)] dE_\rho \quad (2.6.17)$$

The occupancy functions  $f_1$  and  $f_2$  are defined near the interfaces. since the exact shape of these distributions is usually not known, approximate shapes are commonly used. Further more, it is assumed that the distributions are isotropic.

In equilibrium, the energy distribution functions of electrons and holes is given by fermi-dirac statistics  $f(E) = \frac{1}{1 + \exp[\frac{E - E_f}{k_B T}]}$

$E = E_x + E_\rho$  and splitting integrals

$$N(E_x) = \xi_1(E_x) - \xi_2(E_x),$$

The value of  $\xi_1$  and  $\xi_2$  becomes

$$\xi_i = \int_0^\infty f_i(E) dE_\rho = \int_0^\infty \frac{1}{1 + \exp[\frac{E_x - E_\rho - E_{f_i}}{k_B T}]} dE_\rho,$$

where  $i=1,2$

The last expression can be integrated analitically using

$$\int \frac{dx}{1 + \exp(x)} = \ln\left(\frac{1}{1 + \exp(-x)}\right) + c,$$

Then the total supply function is

$$N(E_x) = k_B T \ln \left[ \frac{1 + \exp\left(\frac{E_{f_1} - E_x}{k_B T}\right)}{1 + \exp\left(\frac{E_{f_2} - E_x}{k_B T}\right)} \right] \text{ from the above expression the tunneling current density become}$$

$$J = \frac{q^3 m_{eff}}{8\pi m d \pi \epsilon_d \hbar q \phi_1} E^2 \epsilon_d \exp\left(\frac{-4\sqrt{2m\epsilon_d}(\phi_B^3)}{3\hbar q E \epsilon_d}\right) \quad (2.6.18)$$

. where  $\epsilon_d$  is dielectric constant.

# Chapter 3

## RESULTS AND DISCUSSION

In this section, we will present the relationship between three different parameters determining current density. That is temperature, field emission, dopant density of semiconductor on metal semiconductor interfaces. We have shown our gnuplot result in figure 1,2,3. Based on our gnuplot result, we tried to show the following.

1. The effects of temperature on current density.
2. The effects of external field on current density.
3. The effects of dopant density of semiconductors on current density

### 3.1 The Effects Of Temperature On Current Density

The plot in figure 4.1, shows the relation between current density and temperature with constant work function of Aluminium (4.28 eV) and silicon (4.85 eV). The plot shows current density (J) as a function of temperature (T). If the temperature increases, current density increases exponentially. This means at a constant barrier height, the increasing temperature of metal (Aluminium) and semiconductor (silicon), the emission of electron density increases exponentially or when decreasing temperature with constant barrier height of semiconductor (Silicon) and Aluminium,

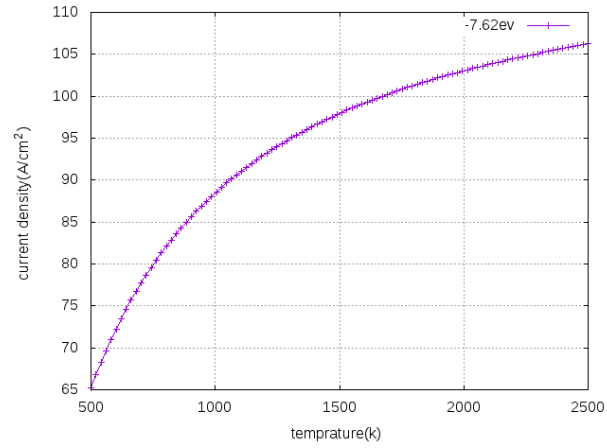


Figure 3.1: Current density versus temperature

the emission of electron density decreases exponentially. This relationship is described by equation (2.3.20).

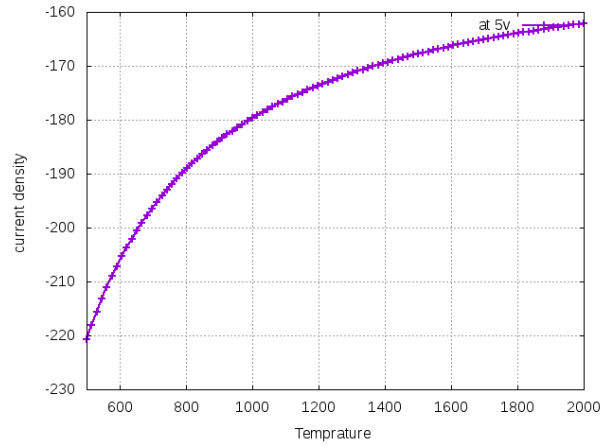


Figure 3.2: Current density as a function of temperature with source voltage ( $V=5v$ )

Figure 4.2 shows, the current density as a function of temperature at constant bias voltage 5V. If the temperature increases, the current density increases exponentially. This relation ship is described by equation (2.5.14).

## 3.2 The Effects Of Forward Bias Voltage On Current Density

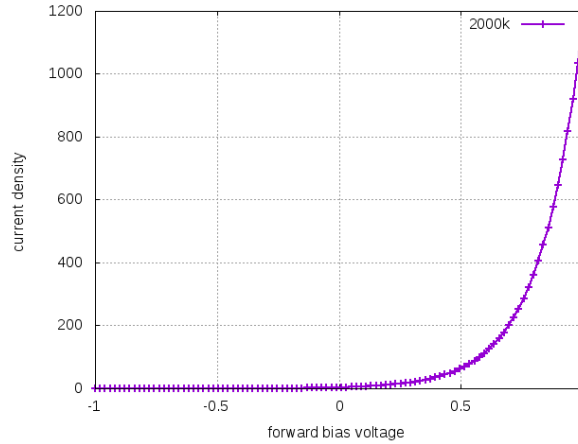


Figure 3.3: Current density as a function of forward bias voltage at constant temperature

From 4.3 we observe , at a constant temperature, when forward voltage increases from -1 ev to 0 ev the current density saturated because the barrier height is large on semiconductor side .so,electro can not jump on a greater barrier. on the other hand,the current density increases exponentially as the forward bias voltage changes from 0ev to 1ev due to small barrier height on semiconductor side. so the saturation current density  $(J_o) = AT^2 \exp(\frac{-q\phi_{Bn}}{K_B T})$  equal to  $4.8 \times 10^8$ ,then the current density  $J = J_o[\exp(\frac{qv_a}{K_B T}) - 1]$ . The saturation current density  $(J_o)$  depends exponentially on barrier height( $\phi_{Bn} = \phi_m - \chi_s = 4.28\text{ev} - 11.9\text{ev} = -7.62\text{ev}$ )and is needed in order to reduce the value of  $(J_o)$  in schottky junction. So, exponential dependency of the current density on both temperature and forward bias voltage

### 3.3 The Effects Of Dopant Concentration On Current Density

The relationship between current density on dopant concentration is described by equation (2.5.11).

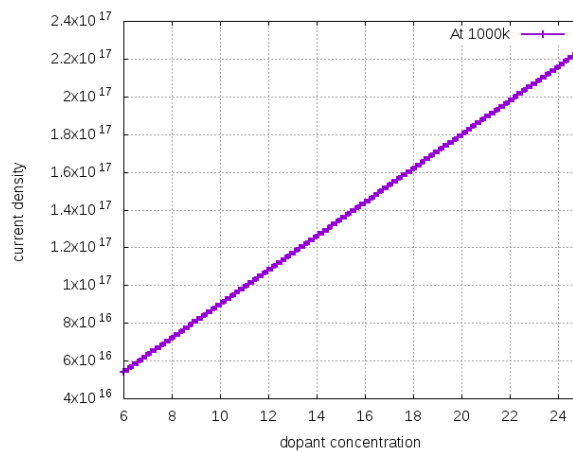


Figure 3.4: Current density as a function of dopant concentration at constant temperature

Fig 4.4 illustrates the effect of dopant concentration on current density at a constant temperature. From this figure we observe that, at a constant temperature the current density directly proportional to the dopant concentration. This means as the dopant concentration of semiconductor increases, the current density increases uniformly and vice-versa.

# Chapter 4

## CONCLUSION

In this project we studied charge transport across metal N-type semiconductor interfaces. To study the charge transport across the interface we have taken N-type silicon and Aluminium interface. The charge (current density) is order parameter of the project. Here we have seen the factors affecting of the current density of metal with N-type semiconductor interface. Temperature, barrier height, image force lowering, field emission, bias voltage and dopant concentration of semiconductor are the major factors of charge transport across the interfaces of metal with N-type semiconductor.

As the temperature of the given interface increases, the current density increases exponentially. Similarly we investigate the relationship of current density and barrier height. Hence, the current density increases as the barrier height decreases when the image force lowers the barrier height. This means the current density indirectly affects by image force lowering. Field emission has the effect in barrier height. The barrier height reduced by increasing field. Note that inside a metal semiconductor interface, the field is not zero even with out bias due to in built in potential. Therefore at high fields the schottky barrier is considerably lowered, and the effective metal work function for thermionic emission reduced.

The forward bias voltage is also another factors affecting of current density. so, if the bias voltage changes from zero to some negative value the current density vanishes.

on the other hand ,for  $v_a > 0$  current density increases exponentially.

Finally we investigated the effects of dopant concentration on current density. Hence, the current density is directly proportional to the dopant concentration of semiconductor. As the dopant concentration increases, the current density increases uniformly.

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## DECLARATION

I,here by declare that this master of science is my original work and it has not been presented for a degree in any other university and that all source of materials used for the thesis has been duly acknowledged.

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