

### 3.4.4. Derivation of the Metal-Semiconductor Junction Current

#### 3.4.4.1. Derivation of the diffusion current

We start from equation (2.10.7) for the total current:

$$J_n = q(\mu_n n \mathcal{E} + D_n \frac{dn}{dx}) \quad (3.4.11)$$

which can be rewritten by using  $\mathcal{E} = -d\phi/dx$  and multiplying both sides of the equation with  $\exp(-\phi/V_t)$ , yielding:

$$J_n \exp(-\frac{\phi}{V_t}) = qD_n (-\frac{n}{V_t} \frac{d\phi}{dx} + \frac{dn}{dx}) \exp(-\frac{\phi}{V_t}) = qD_n \frac{d}{dx} \left[ n \exp(-\frac{\phi}{V_t}) \right] \quad (3.4.12)$$

Integration of both sides of the equation over the depletion region yields:

$$J_n = \frac{qD_n n \exp(-\frac{\phi}{V_t}) \Big|_0^{x_d}}{\int_0^{x_d} \exp(-\frac{\phi}{V_t}) dx} = \frac{qD_n N_c \exp(-\frac{\phi_B}{V_t}) \left[ \exp(\frac{V_a}{V_t}) - 1 \right]}{\int_0^{x_d} \exp(-\frac{\phi}{V_t}) dx} \quad (3.4.13)$$

Where the values listed in Table 3.4.1 were used for the electron density and the potential:

	$n(x)$	$\phi(x)$
$x = 0$	$N_c \exp(-\phi_B/V_t)$	0
$x = x_d$	$N_d = N_c \exp(-\phi_B/V_t) \exp(\phi_i/V_t)$	$\phi_i - V_a$

**Table 3.4.1** Boundary conditions used to solve equation (3.4.13)

The integral in the denominator is solved using the potential obtained from the full depletion approximation solution. Equation (3.3.7) can be written as:

$$\phi = \frac{qN_d}{\epsilon_s} x (x_d - \frac{x}{2}) \cong \frac{qN_d}{\epsilon_s} x x_d = (\phi_i - V_a) \frac{2x}{x_d} \quad (3.4.14)$$

where the second term is dropped since the linear term is dominant if  $x \ll x_d$ . Using this approximation the integral becomes:

$$\int_0^{x_d} \exp(-\frac{\phi}{V_t}) dx \cong x_d \frac{V_t}{2(\phi_i - V_a)} \quad (3.4.15)$$

for  $(\phi_i - V_a) > V_t$ . This yields the final expression for the current due to diffusion:

$$J_n = \frac{qD_n N_c}{V_t} \sqrt{\frac{2q(\phi_i - V_a)N_d}{\epsilon_s}} \exp(-\frac{\phi_B}{V_t}) [\exp(\frac{V_a}{V_t}) - 1] \quad (3.4.16)$$

Where equation (3.3.9) was used for  $x_d$ . This expression indicates that the current depends exponentially on the applied voltage,  $V_a$ , and the barrier height,  $\phi_B$ . The prefactor can be understood physically if one rewrites that term as a function of the electric field at the metal-semiconductor interface (equation (3.3.10),  $\mathcal{E}_{\max}$ :

$$\mathcal{E}_{\max} = \sqrt{\frac{2q(\phi_i - V_a)N_d}{\epsilon_s}} \quad (3.4.17)$$

yielding:

$$J_n = q\mu_n \mathcal{E}_{\max} N_c \exp(-\frac{\phi_B}{V_t}) [\exp(\frac{V_a}{V_t}) - 1] \quad (3.4.18)$$

so that the prefactor equals the drift current at the metal-semiconductor interface, which for zero applied voltage exactly balances the diffusion current.

#### 3.4.4.2. Derivation of the thermionic emission current

The thermionic emission theory<sup>1</sup> assumes that electrons, which have an energy larger than the top of the barrier will cross the barrier, provided they move towards the barrier. The actual shape of the barrier is hereby ignored. The current from the semiconductor to the metal (right to left) is the given by:

$$J_{right-left} = \int_{E_c(x=\infty)+q\phi_n}^{\infty} qv_x \frac{dn(E)}{dE} dE \quad (3.4.19)$$

using (2.4.7) and assuming a non-degenerate doped semiconductor with  $E_{F,n} < E_c - 3kT$ , the density of electrons per unit energy is given by:

$$\frac{dn(E)}{dE} = g_c(E)F(E) = \frac{4\pi(2m^*)^{3/2}}{h^3} \sqrt{E - E_c} \exp[-(\frac{E - E_{F,n}}{kT})] \quad (3.4.20)$$

Assuming a parabolic conduction band (with constant effective mass  $m^*$ ), the carrier kinetic

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<sup>1</sup>see also S.M. Sze "Physics of Semiconductor Devices", Wiley and Sons, second edition, p. 255

energy,  $E - E_c$ , can be related to its velocity,  $v$ , by:

$$E - E_c = \frac{m^* v^2}{2}, \text{ so that } dE = m^* v dv, \text{ and } \sqrt{E - E_c} = v \sqrt{\frac{m^*}{2}} \quad (3.4.21)$$

Combining (3.4.20) with (3.4.21) yields:

$$\frac{dn}{dE} dE = 2 \left( \frac{m^*}{h} \right)^3 \exp \left[ -\frac{E_c(x=\infty) - E_{F,n}}{kT} \right] \exp \left[ -\frac{m^* v^2}{2kT} \right] 4\pi v^2 dv \quad (3.4.22)$$

We now replace  $v^2$  by  $v_x^2 + v_y^2 + v_z^2$  and convert from spherical to Cartesian coordinates by replacing  $4\pi v^2 dv$  by  $dv_x dv_y dv_z$ . The current then becomes:

$$\begin{aligned} J_{right \rightarrow left} &= 2 \left( \frac{m^*}{h} \right)^3 \int_{-\infty}^{\infty} \exp \left[ -\frac{m^* v_y^2}{2kT} \right] dv_y \int_{-\infty}^{\infty} \exp \left[ -\frac{m^* v_z^2}{2kT} \right] dv_z \\ &\quad \int_{-\infty}^{-v_{0x}} q v_x \exp \left[ -\frac{m^* v_x^2}{2kT} \right] dv_x \exp \left[ -\frac{E_c(x=\infty) - E_{F,n}}{kT} \right] \\ &= 2q \left( \frac{m^*}{h} \right)^3 \frac{2\pi kT}{m^*} \exp \left[ -\frac{E_c(x=\infty) - E_{F,n}}{kT} \right] \exp \left[ -\frac{m^* v_{0x}^2}{2kT} \right] \frac{kT}{m^*} \end{aligned} \quad (3.4.23)$$

using<sup>#</sup>:

$$\int_{-\infty}^{\infty} \exp \left[ -\frac{m^* v_y^2}{2kT} \right] dv_y = \int_{-\infty}^{\infty} \exp \left[ -\frac{m^* v_z^2}{2kT} \right] dv_z = \sqrt{\frac{2\pi kT}{m^*}} \quad (3.4.24)$$

The velocity  $v_{0x}$  is obtained by setting the kinetic energy equal to the potential across the  $n$ -type region:

$$\frac{m^* v_{0x}^2}{2} = q\phi_n \quad (3.4.25)$$

so that  $v_{0x}$  is the minimal velocity of an electron in the quasi-neutral  $n$ -type region, needed to cross the barrier. Using

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<sup>#</sup> since  $\int_{-\infty}^{\infty} \exp(-x^2) dx = \sqrt{\pi}$

$$\phi_n = \phi_i - V_a = \phi_B - \frac{1}{q}[E_c(x = \infty) - E_{F,n}] - V_a \quad (3.4.26)$$

which is valid for a metal-semiconductor junction, one obtains:

$$J_{MS} = A^* T^2 \exp\left(-\frac{\phi_B}{V_t}\right) \left[\exp\left(\frac{V_a}{V_t}\right) - 1\right] \quad (3.4.27)$$

where

$$A^* = \frac{4\pi q m^* k^2}{h^3} \quad (3.4.28)$$

is the Richardson constant and  $\phi_B$  is the Schottky barrier height which equals the difference between the Fermi level in the metal,  $E_{F,M}$  and the conduction band edge,  $E_c$ , evaluated at the interface between the metal and the semiconductor. The -1 term is added to account for the current from right to left<sup>2</sup>. The carrier flow from right to left is independent of the applied voltage since the barrier is independent of the band bending<sup>3</sup> in the semiconductor and equal to  $\phi_B$ . Therefore it can be evaluated at any voltage. For  $V_a = 0$  the total current must be zero, yielding the -1 term.

The expression for the current due to thermionic emission can also be written as a function of the average velocity with which the electrons at the interface approach the barrier.

$$v_R = \frac{\int_0^\infty v_x dn(E)}{\int_0^\infty dn(E)}, \text{ including only positive values for } v_x \quad (3.4.29)$$

This velocity is referred to as the Richardson velocity, and is obtained by combining with (3.4.21) and (3.4.22):

$$v_R = \frac{\int_0^\infty v_x \exp\left(-\frac{m^* v_x^2}{2kT}\right) dv_x}{\int_{-\infty}^\infty \exp\left(-\frac{m^* v_x^2}{2kT}\right) dv_x} = \sqrt{\frac{kT}{2\pi m^*}} \quad (3.4.30)$$

So that the current density, equation (3.4.27), becomes:

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<sup>2</sup>This derivation assumes that the effective mass of the carriers is the same on both sides of the barrier.

<sup>3</sup>ignoring the Schottky barrier lowering due to image charges

$$J_n = qv_R N_c \exp\left(-\frac{\phi_B}{V_t}\right) \left[\exp\left(\frac{V_a}{V_t}\right) - 1\right] \quad (3.4.31)$$

where  $N_c$  is the effective density of states, equation (2.6.14).

#### 3.4.4.3. Derivation of the tunneling current

To derive the tunnel current, we start from the time independent Schrödinger equation:

$$-\frac{\hbar^2}{2m^*} \frac{d^2\Psi}{dx^2} + V(x)\Psi = E\Psi \quad (3.4.32)$$

which can be rewritten as

$$\frac{d^2\Psi}{dx^2} = \frac{2m^*(V-E)}{\hbar^2} \Psi \quad (3.4.33)$$

Assuming that  $V(x) - E$  is independent of position in a section between  $x$  and  $x+dx$  this equation can be solved yielding:

$$\Psi(x+dx) = \Psi(x) \exp(-k dx) \text{ with } k = \frac{\sqrt{2m^*(V(x)-E)}}{\hbar} \quad (3.4.34)$$

The minus sign is chosen since we assume that the particle moves from left to right. For a slowly varying potential the amplitude of the wave function at  $x = L$  can be related to the wave function at  $x = 0$ :

$$\Psi(L) = \Psi(0) \exp\left(-\int_0^L \frac{\sqrt{2m^*(V(x)-E)}}{\hbar} dx\right) \quad (3.4.35)$$

This equation is referred to as the WKB approximation<sup>4</sup>. From this the tunneling probability,  $\Theta$ , can be calculated for a triangular barrier for which  $V(x)-E = q\phi_B (1-\frac{x}{L})$

$$\Theta = \frac{\Psi(L)\Psi^*(L)}{\Psi(0)\Psi^*(0)} = \exp\left(-2\int_0^L \frac{\sqrt{2m^*}}{\hbar} \sqrt{q\phi_B(1-\frac{x}{L})} dx\right) \quad (3.4.36)$$

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<sup>4</sup>Named after Wetzel, Kramers and Brillouin

The tunneling probability then becomes<sup>5</sup>:

$$\Theta = \exp\left(-\frac{4}{3} \frac{\sqrt{2qm^*}}{\hbar} \frac{\phi_B^{3/2}}{\mathcal{E}}\right) \quad (3.4.37)$$

where the electric field equals  $\mathcal{E} = \phi_B/L$ .

The tunneling current is obtained from the product of the carrier charge, velocity and density. The velocity equals the Richardson velocity, the velocity with which on average the carriers approach the barrier while the carrier density equals the density of available electrons multiplied with the tunneling probability, yielding:

$$J_n = q v_R n \Theta \quad (3.4.38)$$

The tunneling current therefore depends exponentially on the barrier height to the 3/2 power.

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<sup>5</sup>Using  $\int_0^L \sqrt{1 - \frac{x}{L}} dx = \frac{2L}{3}$