New Physical Formulation of the Thermionic Emission Current at the Heterojunction Interface

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Abstract—**The thermionic emission current for electrons across the heterointerface is classically modeled as the difference between two opposing electron fluxes. Here we have developed a new consistent physical model, which includes the carrier degeneracy and nonideal behavior effects, for thermionic emission current at the heterojunction interface. It is shown that the thermionic emission current at the heterojunction interface can be expressed in a simple closed-form formalism which gives the relations among the average directional thermal velocity of electrons, the conduction band discontinuity, and the carrier activities at both sides of the interface. We also discuss the conditions under which the thermionic emission occurs at the heterointerface.**

I. Introduction

IT IS generally recognized from metal–semiconductor diode theory [1] that the thermionic emission phenomenon at the heterojunction interface is one of the important transport mechanisms for the flow of electron (or hole) current across a heterojunction. The classical thermionic model often neglects the effective mass, degeneracy, and density-of-state effects on both sides of the interface as given by (24) below. In addition, the conventional thermionic emission current is usually modeled as the difference between two opposing electron (or hole) fluxes that do not relate anything about the carriers behavior at (or near) the heterojunction interface.

In this paper, we present a new, simple, but general self-consistent thermionic emission formulation for the carrier transport across a heterojunction interface from an irreversible thermodynamic point of view [2], which includes the nonideal behavior of the carriers around the interface. The correlation between the thermionic emission current and the activities of the carriers shows that the thermodynamic parameters are important to the transport mechanisms that determine the thermionic current. The result presented here gives insight into the thermionic transport problems of the carriers across a heterointerface. We also compare the interesting results with those that appeared in several preceding papers. Finally, the necessary conditions of the thermionic current transport mechanism across the heterointerface are also discussed.

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II. Theory

Consider a one-dimensional (n)GaAlAs/(p)GaAs abrupt emitter–base heterojunction with ohmic contacts at $x = 0$ on the n-side and $x = w$ on the p-side, and with the heterointerface at x_j as shown in Fig. 1(a). The energy band diagram of the junction near forward-biased condition is illustrated in Fig. 1(b), where E_l is the local vacuum level, χ is the electron affinity, E_G is the bandgap energy, E_C is the bottom of the conduction band, E_V is the top of the valence band, E_{Fn} is the electron quasi-Fermi level, E_{Fp} is the hole quasi-Fermi level, $\Delta E_C (= \chi_B - \chi_E)$ is the conduction band discontinuity, ΔE_V is the valence band discontinuity, and x_n and x_p are the space-charge-region edges on the n and p sides, respectively.

Here we will focus our analysis on the consistent derivation of the thermionic emission current across the heterojunction interface. We follow the approach in [3] and [4] and include the Fermi–Dirac statistics. The thermionic emission current across the heterointerface can be expressed as

$$J_n = -A^* T^2 e^{-\phi_B/kT} e^{-V_a^p/kT} \cdot \left[\exp\left(\frac{-q\phi_n(x_j^-)}{kT}\right) - \exp\left(\frac{-q\phi_n(x_j^+)}{kT}\right)\right] \quad (1)$$

where $A^* (= 4q\pi k^2 m^*(x_j^+)/h^3$ for the special case of spherical bands) is the Rechardson's constant and $m^*(x_j^+)$ is the effective mass of the electron in the base region. As pointed out in [3], the A^* and m^* values depend on the band structure of the heterojunction. $\phi_B = E_{GB} - V_p - V_{bi}^p + \chi_B - \chi_E$, where $V_p = E_F^p(w) - E_{VB}(w)$ and V_{bi}^p is the build-in potential across the p-side region. V_a^p represents the portion of the applied voltage that appears across the p-type junction. $\phi_n(x) = [E_F^p(w) - E_{Fn}(x)]/q$ is the quasi-Fermi potentials for the electrons. It should be noted here that quasi-equilibrium condition can be applied at $x = w$. Thus, by convention, we have $E_{Fn}(w) = E_{Fp}(w) \equiv E_F^p(w)$.

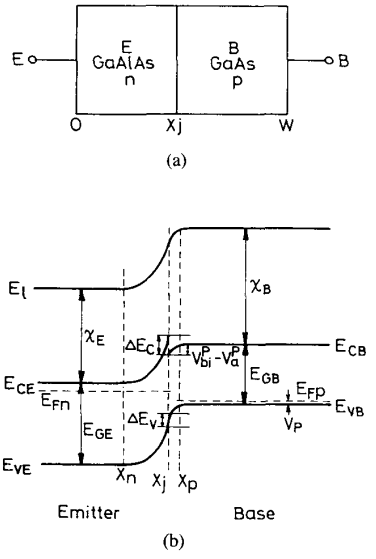

Fig. 1. (a) One-dimensional n-p emitter–base heterojunction device structure; (b) qualitative energy band diagram for (a) under forward-biased condition, including the partial hole and electron quasi-Fermi levels, and the band discontinuities.

If we assume Fermi–Dirac statistics and write the equilibrium electron density as

$$n_0(x) = N_C \exp\left(\frac{E_F - E_C}{kT}\right)\zeta_C \tag{2}$$

after some algebraic manipulation, the thermionic emission current across the junction can be written as

$$J_n = \frac{-qS_{KL}^P n_0(x_{p0})}{\zeta_c(x_{p0})}\exp\left(\frac{qV_{jp} - \Delta E_C}{kT}\right) \cdot\left[\exp\left(\frac{-q\phi_n(x_j^-)}{kT}\right) - \exp\left(\frac{-q\phi_n(x_j^+)}{kT}\right)\right] \tag{3}$$

where $\zeta_C(x)$ $(= F_{1/2}(\eta_C)/\exp(\eta_C))$ is the degeneracy effect for semiconductors with parabolic bands and $F_{1/2}$ is the Fermi–Dirac integral of order one-half with

$$\eta_C(x) = \frac{E_{Fn}(x) - E_C(x)}{kT}. \tag{4}$$

V_{jp} is the potential drop on the p side of the junction and is given by

$$V_{jp} = V_{bi}^p - V_a^p = V(x_j) - V(x_p). \tag{5}$$

$S_{KL}^p (= ([kT/2\pi m^*(x_j^+)])^{1/2})$ is the average directional thermal velocity of electrons (in p-side material) moving in the direction perpendicular to the interface. The subscript zero in (3) denotes equilibrium. Also, we assume that $n_0(W) = n_0(x_{p0})$. This assumption is good for the uniformly heavily doped base band structure [5]. Note that the Fermi–Dirac integral of order one-half $(F_{1/2})$ used here implies that the standard parabolic or spherical band structure is assumed. This is not the general situation for the case of high doping [5]. It is also noted that Fermi–Dirac statistics for the electrons on both sides of the heterointerface are used in the derivation of (1). In addition, the electron temperatures of each side of the interface are assumed to be equal. This implies that the hot-electron injection effects (e.g., ballistic transport and velocity overshoot effects) can be neglected.

The electron concentration in an isothermal compositionally nonuniform degenerate semiconductor can be related to its activity coefficient in the following general form [2]:

$$n(x) = \frac{n_i(w)}{\gamma_n(x)}\exp\left[\frac{q(V(x) - \phi_n(x))}{kT}\right] \tag{6}$$

and

$$\gamma_n(x) = \exp\left(\frac{-A\Delta E_g}{kT}\right) \tag{7}$$

where A is the effective asymmetry factor and ΔE_g is the effective bandgap shrinkage which accounts for the actual bandgap narrowing effect, the density-of-state effects, and the influence of Fermi–Dirac statistics. Here we choose $x = w$ as the reference position for the electrostatic potential. Parameters ΔE_g and A are defined as

$$\Delta E_g = [E_G(w) - E_G(x)] + kT \ln\left[\frac{N_C(x)N_V(x)}{N_C(w)N_V(w)}\right] + kT \ln[\zeta_C(x)\zeta_V(x)] \tag{8}$$

and

$$A = \frac{\left[(\chi(x) - \chi(w)) + kT \ln\left(\frac{N_C(x)}{N_C(w)}\right) + kT \ln(\zeta_C(x))\right]}{\Delta E_g}. \tag{9}$$

The activity coefficient here accounts for the nonideal behavior of the carriers due to heavy doping effects and nonuniform band structure. This coefficient is a function of electron affinity, bandgap, doping density, and the density of states that vary with position. It is important to mention here that, for $A = 1/2$ (symmetric case), (6) is reduced to the conventional degenerate result as [6]

$$n(x) = n_{ie}(x)\exp\left[\frac{q(V(x) - \phi_n(x))}{kT}\right] \tag{10}$$

where $n_{ie}(x)$ is an effective intrinsic carrier concentration as defined in [2]. Generally, this condition (i.e., $A = 1/2$) is not the case for the real systems.

The electron concentration at x_j^- is obtained by putting $x = x_j^-$ in (6) as

$$n(x_j^-) = n_i(w) \cdot \exp\left[\frac{q(V(x_j^-) - \phi_n(x_j^-)) + A\Delta E_g(x_j^-)}{kT}\right]. \tag{11}$$

The intrinsic carrier concentration $n_i(w)$ in (11) can be related to the equilibrium electron concentration at $x = x_{p0}$ in (6) as

$$n_i(w) = n_0(x_{p0}) \exp\left[\frac{-qV^0(x_{p0}) - A\Delta E_g^0(x_{p0})}{kT}\right]. \tag{12}$$

Substituting (12) into (11), followed by some rearrangement, gives

$$n_0(x_{p0}) \exp\left(\frac{-q\phi_n(x_j^-)}{kT}\right) = n(x_j^-) \exp\left[\frac{q\big(V(x_{p0}) - V(x_j^-)\big)}{kT}\right] \cdot \exp\left[\frac{A\Delta E_g(x_{p0}) - A\Delta E_g(x_j^-)}{kT}\right]. \tag{13}$$

In a similar manner, we have the results for the case at $x = x_j^+$ as

$$n_0(x_{p0}) \exp\left(\frac{-q\phi_n(x_j^+)}{kT}\right) = n(x_j^+) \exp\left[\frac{q\big(V(x_{p0}) - V(x_j^+)\big)}{kT}\right] \cdot \exp\left[\frac{A\Delta E_g(x_{p0}) - A\Delta E_g(x_j^+)}{kT}\right]. \tag{14}$$

Furthermore, using the following equations

$$A\Delta E_g(x_{p0}) = kT \ln\left[\zeta_C(x_{p0})\right] \tag{15}$$

$$A\Delta E_g(x_j^+) = kT \ln\left[\zeta_C(x_j^+)\right] \tag{16}$$

$$A\Delta E_g(x_j^-) = -\Delta E_C + kT \ln\left[\frac{N_C(x_j^-)}{N_C(w)}\right] + kT \ln\left[\zeta_C(x_j^-)\right] \tag{17}$$

$$V(x_j^-) = V(x_j^+) = V(x_j) \tag{18}$$

and substituting (5), (13), and (14) into (3), followed by some algebraic manipulations, gives

$$J_n = -qS_{KL}^p\left[\frac{n(x_j^-)}{\zeta_C(x_j^-)}\frac{N_C^p}{N_C^n} - \frac{n(x_j^+)}{\zeta_C(x_j^+)}e^{-\Delta E_C/kT}\right]. \tag{19}$$

Here we assume that $N_C(x_j^-) = N_C^n$ and $N_C(w) = N_C^p$. It should be mentioned here that simple closed-form self-consistent current–voltage characteristics for the carrier transport by drift and diffusion across the space-charge region (conventional model) along with the thermionic emission across the heterointerface (as presented here) can be readily connected and obtained from [2] for the abrupt heterojunction diodes and bipolar transistors with heavily doped concentrations and nonuniform band structure under one-dimensional analysis. The results will be published elsewhere in the future.

Equation (19) can be further rearranged to get the new simple formulation of the thermionic emission current at the heterojunction interface. Two cases will be studied here. First, if we move $e^{-\Delta E_c/kT}$ in the second term of (19) out of the parentheses and use (7), (16) and (17), then we obtain

$$J_n = -qS_{KL}^p e^{-\Delta E_C/kT}\left[n(x_j^-)\gamma_n(x_j^-) - n(x_j^+)\gamma_n(x_j^+)\right] = -qS_{KL}^p e^{-\Delta E_C/kT}\left[a_n(x_j^-) - a_n(x_j^+)\right] \tag{20}$$

where a_n is the activity of the electron and is the product of concentration and activity coefficient. Equation (20) is a new, general, and simple formulation that relates the thermionic emission current to the difference of the electron activity on both sides of the interface. In addition, it is clear from (20) that the magnitude of the J_n is also determined by the average of the directional thermal velocity S_{kL}^p and the conduction band discontinuity ΔE_C. Secondly, if we move $N_C^p/N_C^n\zeta_C(x_j^-)$ in the first term of (19) out of the parentheses and again use (7), (16), and (17), then we have

$$J_n = \frac{-qS_{KL}^n}{\zeta_C(x_j^-)}\left[\frac{m^*(x_j^+)}{m^*(x_j^-)}\right]\left[n(x_j^-) - n(x_j^+)\Gamma(x_j)\right] \tag{21}$$

where

$$S_{KL}^n = \left[\frac{kT}{2\pi m^*(x_j^-)}\right]^{1/2} \tag{22}$$

and

$$\Gamma(x_j) \equiv \frac{\gamma_n(x_j^+)}{\gamma_n(x_j^-)} = \exp\left\{-\left[\Delta E_C + kT \ln\left[\frac{N_C(x_j^+)}{N_C(x_j^-)}\right] + kT \ln\left[\frac{\zeta_C(x_j^+)}{\zeta_C(x_j^-)}\right]\right]/kT\right\} \tag{23}$$

represent the relative nonideal behavior of electrons at the junction interface. Equation (21) represents the general form of the thermionic emission current for electrons across the heterointerface modeled as the difference between two opposing electron fluxes. If we neglect the effective mass, degeneracy, and density-of-states effects on both sides of the interface, then (21) is reduced to

$$J_n = -qS_{KL}^n\left[n(x_j^-) - n(x_j^+)e^{-\Delta E_C/kT}\right]. \tag{24}$$

Equation (24) gives the simplified classical result as that given by Grinberg *et al.* [7]. Apparently, the results presented above can be used to study the band discontinuity.

As is evident from (1), (20), or (21), the necessary conditions of the thermionic current transport mechanism across the heterojunction interface can be readily obtained. For the case of (1) and (2), we have

$$\phi_n(x_j^-) \neq \phi_n(x_j^+) \tag{25}$$

or

$$E_{Fn}(x_j^-) \neq E_{Fn}(x_j^+). \tag{26}$$

From (20) or (21), the condition must satisfy either

$$a_n(x_j^-) \neq a_n(x_j^+) \tag{27}$$

or

$$n(x_j^-) \neq n(x_j^+)\Gamma(x_j). \tag{28}$$

III. Conclusion

This paper reports on some interesting, general, and new formulations of the thermionic emission current across the heterojunction interface. The new results account for the nonideal behavior of electrons on both sides of the interface. In addition, this new physical model is both thermodynamically consistent and consistent with the electronic transport equations. Finally, it should be pointed out that the results presented here are quite general and can also be readily extended to a consistent solution for the case of hole thermionic transport across the valence band heterointerface.

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