An Heterojunction Schottky Barrier Diode with RTD Emitter

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Abstract

The possible application of Schottky diodes as detector elements in receivers and image sensing systems operating in the THz frequency range has been demonstrated in the literature. In addition to metal-semiconductor (M-S) Schottky diodes, the use of heterojunction Schottky barrier diodes for detection and mixing applications has also been explored. Such diodes require lower d.c. bias voltages, which is important for certain types of detector and mixer designs which strive to achieve higher signal-to-noise ratios.

A new detector design is proposed which utilizes a heterojunction Schottky barrier and a double barrier structure jointly for high sensitivity detection. The diode is designed so that the resonant energy level of the double barrier structure is lower than the Schottky barrier at low bias and becomes higher than the barrier as bias increases. In this regime, the thermo distribution of emitted electrons is altered by the presence of double barrier structure, leading to a sharp knee point and a significant improvement in sensitivity.

As compared with a "plain" heterojunction Schottky diode, high frequency response will be affected by the tunneling time through the RTD in addition to the capacitance from junction itself. Such high frequency influences are discussed.
I. INTRODUCTION

The potential application of heterojunction Schottky barrier diodes as mixer and detector elements for the THz frequency range has stimulated interest because of lower possible turn-on voltage, which in turn leads to a lower LO power requirement [1]. In much of the recent literature, the heterojunction Schottky barrier has been treated as an extension of a metal-semiconductor (M-S) Schottky junction. In this case, a generalized model of carrier transport through the heterojunction is used which considers drift-diffusion as well as thermionic emission. In the analysis of Wu and Yang [2] and also Bhapkar [3], quantum mechanical tunneling is considered which includes the current contribution from electrons with energy lower than the barrier height. Applying quantum mechanical modeling to heterojunction Schottky barrier diodes becomes attractive because it not only allows better understanding and modeling of the transport process across the heterojunction (which is important for HEMT and HBT devices), but also allows exploration of more complicated MBE grown heterostructures.

While the I-V curve of a heterojunction Schottky barrier diode is very similar to its M-S counterpart, an intrinsic complexity stems from the non-degenerate character of electron gases on both sides of the interface. In general, the solution of Poisson equation is needed to first obtain the potential profile in the heterojunction region under various bias voltages. Once these potential profiles are determined, the current density can then be calculated using the transmission coefficient method as shown in [3].

In this paper, the current through the heterojunction is computed using the transmission coefficient method of Wu and Yang for such parameters as bias voltage, barrier height, electron density, etc. This method is then applied to the new diode structure proposed here, namely a design utilizing a double barrier quantum filter adjacent to the heterojunction. Since the double barrier structure blocks electrons from tunneling through except at selected energies, the I-V character of the diode is altered dramatically. This novel I-V characteristic will be computed and then compared to a diode without the double barrier structure.
II. CURRENT COMPUTATION

The boundary condition for electron current across a M-S interface as given by Crowell and Sze [4] is:

\[ J = q(n_s - n_0)v_{rn} \]  \hspace{1cm} (1)

where \( n_s \) is the electron density present at the potential maximum and \( n_0 \) is the electron concentration at the same point at equilibrium. In Eq. (1), \( n_s \) can also be defined as the density in the bulk region if we notice that:

\[ n_s = N_0 \exp\left(\frac{E_f - V}{kT}\right) = n_{s,bulk} \exp\left(-\frac{V}{kT}\right) \]  \hspace{1cm} (2)

applies under the Boltzmann distribution assumption. Also, it is straightforward to think of \( qv_{rn}n_0 \) as the current injection from the metal to the semiconductor side, due to the fact that at equilibrium the net current flow is zero. Thus, the current can be written as \( J = J_{sm} - J_{ms} \) where \( J_{sm} \) is the current flux from semiconductor to metal side, while \( J_{ms} \) is the current flux from metal to semiconductor side.

For a heterojunction Schottky barrier, a similar result has been given in Ref. [2] based on the transmission coefficient approach:

\[ J = q\eta(n_1v_1 - \theta n_2v_2)\exp\left(-\frac{E_B}{kT}\right) \]  \hspace{1cm} (3)

where \( n_1 \) and \( n_2 \) are the electron densities on side-1 and side-2 of the interface, \( E_B \) is the energy difference between bottoms of conduction bands on the two sides, and \( \theta \) accounts for the ratio of the effective masses, that is \( \theta = m_1/m_2 \). Furthermore, the effective recombination velocities for each side are given as \( v_1 = A_1^*/qN_{c1} \) and \( v_2 = A_2^*/qN_{c2} \), where \( A_1^* = (qm_1^*k^2/2\pi^2\hbar^3) \) and \( A_2^* = (qm_2^*k^2/2\pi^2\hbar^3) \) are the Richardson constants for each side. Also in Eq. (3), \( \eta \) is a term which comes from the integration over the transmission coefficient and the distribution functions. Specifically, it is computed as:

\[ \eta = \int_{\max(E_B,0)}^{\infty} dE_||\exp\left(-\frac{E_||}{kT}\right) \int_{0}^{(E_B-E_||)/(1/\theta-1)} dE_\perp T(E_||, E_\perp)\exp\left(-\frac{E_\perp}{kT}\right) \text{ if } \theta < 1 \]  \hspace{1cm} (4)

\[ = \int_{0}^{\infty} dE_||\exp\left(-\frac{E_||}{kT}\right) \int_{\max((E_B-E_||)/(1-1/\theta),0)}^{\infty} dE_\perp T(E_||, E_\perp)\exp\left(-\frac{E_\perp}{kT}\right) \text{ if } \theta > 1 \]  \hspace{1cm} (5)
where \( E_{||}, E_\perp \) are the energy components corresponding to electron motion parallel to and perpendicular to the heterojunction interface, respectively. As shown by Horio [6], the classical thermionic emission situation (no tunneling) can be described by assuming that the transmission coefficient takes the form:

\[
T(E_{||}, E_\perp) = \Theta(E_\perp - \Delta \phi)
\]

where \( \Theta \) is the Heavyside step function. Eq. (6) shows that only those electrons with \( E_\perp \) greater than the barrier height can cross the interface without being blocked and thereby contribute to the current. A substitution of \( T \) from Eq. (6) into Eq. (5) will lead to an analytic \( \eta \) in the simple form of:

\[
\eta = T^2 \exp\left(-\frac{\Delta \phi}{kT}\right)
\]

Without loss of generality, this calculation assumes that side-1 is GaAlAs, and that side-2 is GaAs. Thus \( \theta \) (from Eq. (5)) is always greater than 1. Also, consistently with this notation, \( E_B < 0 \) for forward bias.

Using the \( \eta \) given in Eq. (7), the current density in Eq. (3) can be readily identified with M-S Schottky barrier results. However, unlike the M-S Schottky barrier, \( \Delta \phi \) in heterojunction-based diodes generally does not have a linear dependence on bias voltage even at low bias due to the non-degenerate character of material on either side. This leads to less ideal I-V curves as compared with what given by M-S Schottky diodes.

### III. HETEROJUNCTION DIODE MODELING

In order to calculate the barrier height variation as a function of the applied bias voltage, first we solve the Poisson equation to obtain the band profile near the heterojunction region. Only one species of carrier, namely the electron, is considered and thus the Poisson equation becomes:

\[
\frac{d^2 \phi}{dx^2} = -\frac{q}{\varepsilon}(-n + N_d)
\]
where \( N_d \) is the donor density in the device bulk region, \( n = n_i \exp\left(-\frac{E_f-E_c-a(x)}{kT}\right) = N_c \exp\left(-\frac{a(x)}{kT}\right) \) is the electron density in the conduction band, \( E_f \) is the electron Fermi energy, \( E_c \) is the position of conduction band, and \( N_c \) is the density of state in the conduction band. This computation was applied to the device shown in Fig. 1 and the resulting conduction band profiles for three different biases are plotted in Fig. 2. The barrier height bias voltage dependence, \( \Delta \phi - V \), extracted from this calculated band structure is plotted in Fig. 3. As can be seen in the figure, this dependence is approximately linear but it does exhibit a slight non-linear dependence due to the non-degenerate character mentioned previously. Moreover, note that the \( \Delta \phi - V \) term is less then one, due to an applied voltage drop over series resistances in the other parts of the device. However, as can be observed from the plot, the change of the depth of the well on the GaAs side (refer to Fig. 2, where it is noted as \( \Delta \phi_{GaAs} \)), is relatively small, as a result of the relatively heavy doping on the GaAs side as compared with the GaAlAs side.

Knowing the potential profile around the heterojunction region, the quantum mechanical transmission coefficient can be calculated. In this paper, the transmission line technique of Khondker et al [5] is used to calculate the transmission coefficient. The first step in the method is to approximate the conduction band profile within the entire region under consideration by a series of voltage steps, named \( V_i(x_i, x_{i+1}) \), \( i = 1 \ldots N \). Next the corresponding “load impedance” \( Z_i \) and the “characteristic impedance” \( Z_0 \) is iteratively computed through each step. The reflection coefficients and transmission coefficients are obtained from these impedances using the forms:

\[
\rho = \frac{Z_{iN} - Z_0N}{Z_{iN} + Z_0N} \quad (9)
\]

\[
T = 1 - |\rho|^2 \quad (10)
\]

where \( Z_{iN} \) is the load impedance and \( Z_0N \) is the characteristic impedance for step \( N \). Since the transmission coefficient calculation depends only on the energy in the perpendicular direction, the integration in Eq. (5) degenerates to one dimension, and thus becomes:
\[
\eta_q = kT \int_0^\infty dE_\perp T(E_\perp)e^{\frac{-E_\perp}{kT}} \text{ if } \theta > 1
\] (11)

As compared to Eq. (6), this quantum mechanical transmission coefficient will be somewhat larger than zero for energy lower than the barrier height because of the inclusion of a tunneling contribution in the overall transport current. It also leads to a less than one transmission probability for an electron with energy larger than the barrier height due to the scattering by the barrier. The \( \eta_Q \) calculated from Eq. (11) is plotted in Fig. 4, and also included in this plot is the \( \eta_C \) which is the same value calculated from the classical approximation discussed earlier. This plot clearly shows quantum effects characteristic of the problem. For example, at low bias \( \eta_Q \) is little larger than \( \eta_C \) since the tunneling portion of the current is, of course, neglected in the classical approximation. At higher bias, \( \eta_C \) is larger than \( \eta_Q \) since the quantum model takes scattering into account.

IV. EXAMPLE CALCULATION

In the sample device used for computations (Fig. 1), the barrier width at \( E = 0 \) is about 1000Å (Fig. 2), thus the tunneling effect is not very important. However, if the GaAlAs side where more heavily doped, then the barrier would become thinner and the tunneling effect would be more significant.

The GaAlAs/GaAs heterojunction structure modeled here is intended to be used as THz detector, thus current density (e.g. power handling) is not a stringent device performance requirement. For the Schottky barrier heterostructure under consideration, it is possible to further modify the I-V characteristics by adding a superlattice structure next to the heterojunction interface as shown in Fig. 1. A similar approach has been used in the RTD design to reduce the series resistance coming from the ohmic contact by replacing it with a Schottky barrier. At low bias, the resonant energy is lower than the Schottky barrier, and the current is small due to the blocking of barrier. As the voltage increases, the resonant energy gradually approaches the top of Schottky barrier and eventually becomes higher than the barrier height. At this turning point, there is a sharp, steep increase in the current.
as compared with the ideal/classical diode I-V curve. Note that the potential profile as obtained from the solution of Poisson equation is used in this computation.

The calculated \( \eta_Q \) for this structure is plotted in Fig. 5, and the curve indeed shows a sharp knee point around 40meV. As the bias voltage increases, the current response sharply turns on and then sustains a rapid increases, implying much higher possible detector gains for small signals. The original result also shows several small "bumps", especially in the mid-bias region, which come from resonances between the Schottky barrier and the double barrier structure. Although these are indeed accounted for in the modeling, their amplitudes are invariably very weak, and therefore there is virtually no practical implication and is smoothed out. Now, as the voltage increases further, the major part of voltage drop is over the double barrier structure region, which finally leads the diode to negative differential conduction behavior.

One key "circuit-level" parameter which characterizes the detector performance is the open circuit sensitivity, described by:

\[
\beta = \frac{1}{2} \frac{f''(v_0)}{f'(v_0)^2}
\]  \hspace{1cm} (12)

where \( f(v) \) is the I-V relation of the device. For the device parameters under discussion including an assumed device area of 10\( \mu \)m\(^2\), \( \beta \) is estimated to be 63888 (mV/mW) for an applied bias of 0.04V. This compares with \( \beta = 2500\text{mV/mW} \) (based on the thermionic theory calculation) for an conventional same size diode biased at same voltage. The current density is estimated to be \( 1.5 \times 10^{-2} \text{mA\mu m}^{-2} \), which is only fractionally smaller than the current density in an ideal Schottky barrier diode. The series resistance from the bulk regions and the ohmic contacts where not considered in this calculation, thus the results shown here are somewhat optimistic. However, using the methods presented here the series resistance is estimated to be about 60\( \Omega \), which would not greatly degrade the device performance.
V. OTHER CONSIDERATIONS AND CONCLUSIONS

The overall detection efficiency is also greatly affected by the reactive behavior of the diode. For the Schottky barrier portion (i.e., contacts) of the overall structure, the major reactive contribution is capacitive, while in the double barrier device portion the situation is more complicated. For a double barrier region it has been shown that the reactance could be either capacitive or inductive depending on the frequency of operation and device parameters. Although such reactive behavior is not yet fully characterized via current research [8], it is known generally that when the resonant level electron charge density variation is large and the signal frequency is comparable with the inverse of tunneling time (e.g. $1/\tau$), then the diode's behavior becomes inductive. This observation explains why the inductance increases with barrier thickness and why inductive effects are more pronounced when the diode is biased in the NDC region. For the device structure under consideration, the barrier is relatively thin and the device is operated at low bias, therefore the inductance is expected to be small. However, since the intended operation is at very high frequencies (i.e. approaching 1 THz), this inductance still has a finite influence. Since it is of importance, this inductance was estimated to be less than $10^{-2}$nH. The capacitance of the heterojunction is also of importance as well, of course, and it is given by $C_j = A\varepsilon_s/w$ where $A$ is the device area and $w$ is the width of the depletion layer. A 0.04V bias voltage and $w = 0.11\mu$m leads to $C_j \approx 10^{-2}$pF.

From the junction capacitance and the series resistance, the time constant for the overall device is estimated to be $\tau = R_sC_j = 4$ps. Here the inductances from double barrier region and Schottky contacts were not considered. Since the impedance stemming from these inductances is comparable to that from the junction capacitance at the frequency of 1 THz, this would present a formidable simulation task.
REFERENCES

1 X.J. Lu is a postdoc fellow from National Research Council, Washington, D.C.


\[
\begin{align*}
&n^+ \text{Al}_{0.2}\text{Ga}_{0.8}\text{As}(7 \times 10^{18}) \quad 1000\text{A} \\
&n \text{Al}_{0.2}\text{Ga}_{0.8}\text{As}(2 \times 10^{16}) \quad 500\text{A} \\
&\text{AlAs} \quad 7\text{A} \\
&n \text{Al}_{0.2}\text{Ga}_{0.8}\text{As}(2 \times 10^{16}) \quad 60\text{A} \\
&\text{AlAs} \quad 7\text{A} \\
&n \text{Al}_{0.2}\text{Ga}_{0.8}\text{As}(2 \times 10^{16}) \quad 250\text{A} \\
&n \text{GaAs}(1 \times 10^{17}) \quad 400\text{A} \\
&n^+ \text{GaAs}(5 \times 10^{18}) \quad 1000\text{A} \\
\end{align*}
\]

Fig. 1 Cross-section of the heterojunction Schottky barrier diode, and schematic drawing of the detector.
Fig. 2 The band profiles of Schottky heterojunction under various bias voltages.
Fig. 3 The variation of Schottky barrier height vs. the bias voltage increase.
Fig. 4 Modification factor calculated using quantum mechanical transmission coefficient method $\eta_q$ and from thermionic theory $\eta_c$. 
Fig. 5 The modification factor for the Schottky barrier diode with RTD on the emitter side.