Modeling the C-V Characteristics of Heterodimensional Schottky Contacts

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Abstract

This paper addresses the capacitance-voltage (C-V) characteristics of heterodimensional Schottky diodes, in which the Schottky metal is placed in direct contact to a two-dimensional electron gas and the confined electron behavior directly dictates the device performance. We develop a novel quasi-2D model for the C-V characteristics of the device, by starting from a self-consistent solution of the Schrödinger and Poisson equations in the growth direction. The model is validated by contrasting the theoretical results with experimental data from an AlGaAs/GaAs device fabricated in our laboratory.

1. Introduction

The properties of electrons in an inversion layer have attracted interest since the 1930’s, when Lilienfeld conceived the field-effect transistor. Further attention has been motivated by the enhanced transport properties of the two-dimensional electron gas (2-DEG) formed at modulation doped heterointerfaces, where the inversion layer is quantized in the growth direction. Already in the early 90’s High Electron-Mobility Transistors (HEMTs) based on this principle displayed power amplification well above 100 GHz with outstanding noise performance.

This paper is concerned with devices based on a further extension of the modulation doping concept by using heterodimensional interfaces, i.e., interfaces between materials of dissimilar dimensions. In our specific case, this interface is a Schottky barrier laterally connecting a three-dimensional (3D) metal and a two-dimensional (2D) electron gas.

In fact, heterodimensional diodes, transistors and photodetectors present several attractive features such as low capacitance due to the small effective cross-section, excellent noise and transport characteristics due to the 2D electron gas and a high breakdown voltage, making them very promising for high-frequency applications [1-2].

In order to illustrate the motivation for studying heterodimensional devices we briefly revisit the question of computing the thermionic emission current in such devices. In fact, straightforward extension of Bethe’s theory, considering both the proper two-dimensional density of states as well as energy quantization in the growth direction for a 2-DEG with only one significantly populated subband, yields [3]:

\[
J_n = A_{2D}^* T^{3/2} \exp\left(\frac{q\Phi_B}{kT}\right) \exp\left(-\frac{E_0}{kT}\exp\left(\frac{qV}{kT}\right) - 1\right) \tag{1}
\]

where \(A_{2D}^*\) is the two-dimensional equivalent of the Richardson constant [3], \(E_0\) is position of the first allowed energy level in the 2-DEG and the other terms have their usual meanings. Fig 1 computes the ratio given by eq. 2 for a typical AlGaAs/GaAs structure (see section 4) as a function of both the doping density and thickness of the AlGaAs layer, values of \(E_0\) were calculated using the model described in detail in section 3. The large values achieved represent a strong suppression of thermionic emission current, essentially due to the exponential term in \(E_0\). This term acts as an effective Schottky barrier enhancement due to energy level quantization. In fact, despite the simplifications involved in Bethe’s formalism, there are experimental data available [3-4] to support the above predictions by demonstrating one order of magnitude improvement in dark current. By itself, this feature certainly makes heterodimensional structures very attractive as low noise photodetectors as well as low leakage gate contacts.

Despite this vast amount of device-related work, the number of investigations on the modeling of the capacitance-voltage characteristics heterodimensional structures is still limited. In the next sections, we develop a novel quasi-2D model for the C-V characteristics of the device, by starting from a self-consistent solution of the Schrödinger and Poisson}

\[
r = \frac{I_{3D}}{I_{2D}} = \frac{W}{h} \sqrt{\frac{m^*}{2\pi n_0 kT}} \exp\left(\frac{E_0}{kT}\right) \tag{2}
\]

where \(W\) is the effective length of the Schottky contact for a conventional device, typically around 1 µm and the other terms have their usual meanings. Fig 1 computes the ratio given by eq. 2 for a typical AlGaAs/GaAs structure (see section 4) as a function of both the doping density and thickness of the AlGaAs layer, values of \(E_0\) were calculated using the model described in detail in section 3. The large values achieved represent a strong suppression of thermionic emission current, essentially due to the exponential term in \(E_0\). This term acts as an effective Schottky barrier enhancement due to energy level quantization. In fact, despite the simplifications involved in Bethe’s formalism, there are experimental data available [3-4] to support the above predictions by demonstrating one order of magnitude improvement in dark current. By itself, this feature certainly makes heterodimensional structures very attractive as low noise photodetectors as well as low leakage gate contacts.
equations in the growth direction. The model is used as a design guideline and validated by contrasting the theoretical results with experimental data from an AlGaAs/GaAs heterodimensional varactor device fabricated in our laboratory.

2. Capacitance-voltage modeling

The formulations available in the literature to study the electronic properties and capacitance-voltage characteristics of heterodimensional Schottky contacts can be be divided in two classes. In one hand, Gelmont and collaborators [5] extended the original work from Petrosyan and Shik [6] to obtain, by using the conformal mapping technique, an analytical expression for the junction capacitance between a bulk p-type semiconductor and a two-dimensional electron gas. Unfortunately, their expression identically vanishes when the p-type semiconductor is replaced by a metal. Furthermore, the obtained solution does not explicitly accounts for neither the layer structure nor the conduction band diagram, i.e., the potential profile in the growth direction.

On the other hand, fully numerical techniques are also available. Such implementations can use either the Boundary Element Method [7] or the Finite Element Method [8] for the resolution of the Schrödinger and Poisson equations. Nevertheless both methods are very time consuming from the computational point of view they often do not yield self-consistent solutions. Although the problem of interest here is intrinsically bidimensional, due to the presence of the lateral Schottky terminal, usually only the Poisson equation is solved in two dimensions. The Schrodinger equation is still written as a function of the growth direction.

The novel method proposed in this work is an attempt to combine the features of both classes of formulations discussed above. In the next section, we use the analytical description proposed by Petrosyan to represent the longitudinal potential \( V(y) \) along the 2-DEG channel [6] in order to develop an quasi two-dimensional extension of the self-consistent Schrodinger-Poisson solver presented by the authors in reference [9]. In this way, it is possible to explicitly incorporate the layer structure in the formulation. However, the computational effort is much smaller than required by fully numerical techniques [7-8].

3. Theoretical formulation

The model presented in this section is a quasi two-dimensional extension of a work previously published by the authors [9]. We start by self-consistently solving Schrödinger and Poisson equations in the growth direction. The quantum-mechanical formalism is based on the effective mass approximation, where the electron wavefunction is taken as the product of a Bloch function and an envelope function, solution of the time-independent Schrödinger equation:

\[
H \psi_i(x) = E_i \psi_i(x)
\]

The utilized Hamiltonian is able to account position-dependent effective mass and lattice constant and is given by [9]:

\[
H = -\frac{\hbar^2}{2\alpha(x)} \frac{d}{dx} \left[ \frac{a(x)}{m^*} \frac{d}{dx} \right] + V_{ef}(x)
\]

where the potential \( V_{ef} \) includes not only the band-diagram discontinuities and the Hartree term due to the electrostatic potential but also an exchange-correlation term as well as strain components caused by lattice mismatch due, for example, to the insertion of an InGaAs pseudomorphic layer in between the AlGaAs/GaAs heterojunction [9].

The Poisson equation, which yields the above mentioned Hartree term, is given by:

\[
\frac{d}{dx} \left( \varepsilon(x) \frac{d}{dx} \right) V_H(x) = -q \left[ N^+ D^+ - N^+ - n(x) \right]
\]

where \( q \) is the electronic charge, \( \varepsilon(x) \) is the position dependent dielectric constant of the semiconductor, \( N^+ \) is the ionized donor concentration, \( N^+ \) is the ionized non-intentional background acceptor concentration and \( n(x) \) is the free-electron concentration in the conduction band (the free hole concentration has been neglected). We write \( n(x) \), in terms of the electronic eigenfunction \( \psi_i(x) \), as:

\[
n(x) = \frac{m^*_e k T \sum_i}{\pi \hbar^2} \ln \left[ 1 + \exp \left( \frac{E_i - E_F}{k T} \right) \right] |\psi_i(x)|^2
\]

where \( m^*_e \) is the electron effective mass in the 2-DEG channel, \( k \) is the Boltzmann constant, \( T \) is the absolute
temperature, $h$ is the reduced Planck constant, $E_i$ is the Fermi level energy and $E_F$ represents the $i$-th eigenvalue. The Fermi-level position $E_i$ is computed from the usual charge neutrality condition in the bulk material and the above formulation (eqs. 3-6) must be solved self-consistently in real space. In particular, the eigenstates of the Schrödinger equation are numerically calculated by using a split-operator algorithm through a non-uniform finite difference discretization scheme [9], under the boundary conditions that the wavefunction must vanish at the substrate and at the device top surface. The boundary conditions for the Poisson equation are given by the surface potential $V_s$ at the top of the device (taken as $x = 0$) as well as by the position of the conduction band with respect to the Fermi-level in the bulk semiconductor, presenting a non-intentional background ionized doping density $N_A$.

Now, the above formulation is used as an input to develop a novel quasi two-dimensional model for the capacitance-voltage characteristics. Specifically, the y-component of the potential distribution along the channel, $V(y)$, is taken into account considering that, if the sheet electron density $n_s$ into the 2-DEG channel is a function of the surface potential $V_s$ in the general form:

$$ n_s = f(V_s) \quad (7) $$

then the introduction of the longitudinal potential $V(y)$ modifies the carrier distribution along the channel to yield [10-11]:

$$ n_i(y) = f(V_s - V(y)) \quad (8) $$

with the same functional dependence as in eq. (7). Accordingly, in our procedure, for a given terminal voltage, the channel is initially divided into several segments of length $dy$. Next, the capacitance contribution of each segment is computed by solving the one-dimensional Schrodinger-Poisson problem in the growth direction (eqs. 3-8), but now under an “effective” surface potential $V_s = V_s - V(y_i)$, where $y_i$ is a coordinate position located in middle of each segment $dy$. A quasi-static approach was used, giving the capacitance per unit area as the total charge variation caused by a small voltage change around a given bias point. Then, this free-carrier capacitance, $C_{free}$, is given by the summation of the capacitance contribution for each segment $dy$.

4. Device fabrication and experimental validation

In order to verify our model the theoretical predictions were compared to the experimental data of a control AlGaAs/GaAs heterodimensional device fabricated in our labs. The fabrication procedure is given as follows. On top of a buffer layer grown on semi-insulating GaAs substrate, 5000 Å of undoped GaAs was deposited, followed by 100 Å of undoped Al$_{24}$Ga$_{76}$As and 500 Å of 3x10$^{17}$ cm$^{-3}$ n-type Al$_{24}$Ga$_{76}$As. The topmost layer is 200 Å of 3x10$^{18}$ cm$^{-3}$ n-type GaAs layer. All growth was done by molecular beam epitaxy (MBE) and the structure was chosen to be compatible with enhancement type HEMTs where the n+ cap layer is usually used for ohmic contact formation. A trench was formed by wet chemical etching through the Al$_{24}$Ga$_{76}$As layers and 500 Å of Schottky Ti/Au contact metal was deposited on the GaAs side to form Schottky junctions with the 2DEG. The contacts have the usual interdigital MSM structure for a total device area of a total area of 40 μm x 40 μm.

The capacitance-voltage characteristics of the device were measured by directly probing the three terminals and recording the results by a HP LCR meter. It should be noted that independently of the physical mechanism responsible for charge modulation by the applied bias, if the voltage is high enough to fully deplete the semiconductor the capacitance between the electrodes will reach a strictly geometrical lower value, $C_p$, as described in reference [12]. Therefore, the overall capacitance $C_T$ is given by:

$$ C_T = C_{free} + C_p \quad (9) $$

In what follows the $C_p$ value, of about 29 fF for our structure, is already extracted from the experimental data and the discussion is concerned only with the free electron contribution to the device capacitance.

Fig. 2 displays the free-carrier capacitance as a function of the terminal voltage for a heterodimensional Schottky-ohmic device. In order to obtain the theoretical results we used the method described in the previous section, employing the Petrovyan approximation for the longitudinal potential $V(y)$ and simulated exactly the
same layer structure discussed previously, assumed to 
subjected to a surface potential of 0.75V, due to surface 
states causing Fermi-level pinning at the AlGaAs/air 
interface.

The theoretical results obtained are quite satisfactory. 
It is clearly seen that our model was able to reproduce, 
without any fitting parameter, the general features of the 
varactor C-V characteristics, yielding capacitance 
values in the measured range. Given the uncertainty on 
some device parameters (such as the amount of non-
intentional doping at the GaAs buffer layer and value of 
the surface potential at the top of the structure) no 
attempt will be made in this paper to strictly match 
theory and experiment. However, due to satisfactory 
results obtained above, we believe that this novel model 
is an useful tool to optimize the device performance, by 
providing useful design guidelines.

![Figure 3. Dynamic range versus AlGaAs layer thickness as a function of interelectrode spacing for an heterodimensional MSM varactor.](image)

For example, on the basis of figure 2, it is possible to 
define a figure of merit for the dynamic range of the 
device acting as a varactor:

$$\Delta C = C(V=0 \text{ volts}) - C_g$$  \hspace{1cm} (10)

Figure 3 displays the simulated results for $\Delta C$, 
normalized to the contact width of a MSM varactor 
structure, as a function of the AlGaAs layer thickness 
for several values of interelectrode spacing. All the 
remaining parameters were kept unchanged from the 
fabricated device. Interesting enough, apart from 
numerical fluctuations, we verified a linear relationship, 
which considerably simplifies the device design process.

5. Conclusions

A novel model for the C-V characteristics of the 
heterodimensional Schottky contacts was developed. 
The model was validated by comparison with 
experimental data from an AlGaAs/GaAs device and it 
was shown to be an useful tool for varactor design.

6. References

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