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Self-consistent vertical transport calculations in $Al_xGa_{1-x}N$/GaN based resonant tunneling diode

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ABSTRACT

The formation of two-dimensional electron gases (2DEGs) at $Al_xGa_{1-x}N$/GaN hexagonal double-barriers (DB) resonant tunneling diodes (RTD) is investigated by numerical self-consistent (SC) solutions of the coupled Schrödinger and Poisson equations. Spontaneous and piezoelectric effects across the material interfaces are rigorously taken into account. Conduction band profiles, band edges and corresponding envelope functions are calculated in the $Al_xGa_{1-x}N$/GaN structures and likened to those where no polarization effects are included. The combined effect of the polarization-induced bound charge and conduction band offsets between the hexagonal AlGaN and GaN results in the formation of 2DEGs on one side of the DB and a depletion region on the other side. Using the transfer matrix formalism, the vertical transport (J–V characteristics) in AlGaN/GaN RTDs is calculated with a fully SC calculation in the ballistic regime. Compared to standard calculations where the voltage drop along the structure is supposed to be linear, the SC method leads to strong quantitative changes in the J–V characteristics showing that the applied electric field varies significantly in the active region of the structure. The influences of the aluminum composition and the GaN(AlGaN) thickness layers on the evolution of the current characteristics are also self-consistently investigated and discussed. We show that the electrical characteristics are very sensitive to the potential barrier due to the interplay between the potential symmetry and the barrier height and width. More interestingly, we demonstrate that the figures of merit namely the peak-to-valley ratio (PVR) of GaN/AlGaN RTDs can be optimized by increasing the quantum well width.

1. Introduction

III-Nitrides are one of the most interesting semiconductors for the microelectronics industry. They are the materials of choice for ultraviolet blue-green optoelectronics and they hold the potential to complement and even challenge silicon in a number of electronic applications [1]. The main reason for this enthusiasm in (Al, Ga, In)N compounds stems from their direct band gap tunable along a wide range of energies. In this context, AlGaN/GaN heterostructures are good candidates for high power and high frequency amplifying devices for communication. Besides, due to the high energy of their longitudinal optical

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phonon modes (around 92 meV in*GaN*), nitride semiconductors should enable the realization of quantum cascade lasers (QCLs) operating at room temperature in the THz frequency range.

Recent advances in digital and analog systems demand very high performance electronic circuits. Resonant tunneling diodes (RTDs) which display a Negative Differential Resistance (NDR) present very attractive characteristics [2] such as high intrinsic cut-off frequency (in the THz range). The RTD specificities are exploited in digital applications ("multi-value" logic) as well as in analog applications (ADC, frequency divider or multiplier, oscillator), leading to simpler circuits, with a large gain in power consumption and high frequency performance [3,4]. Thin barrier RTDs are specially promising for high frequency generation due to their extremely high speed transport properties with characteristics in order of a few picoseconds [5]. Due to their large conduction band offset (1.75 eV between *AlN* and *GaN*) [6], *GaN* based RTDs should permit to obtain higher voltage and power operation in comparison with conventional III-V semiconductors. However, the wurtzite $Al_xGa_{1-x}N/GaN$ heterostructures possess strong polarization charges at the heterointerfaces making difficult the modeling of vertical electronic transport in RTDs devices. Only limited theoretical studies have been performed on $Al_xGa_{1-x}N/GaN$ RTDs [6–8]. Moreover, the reported electronic characteristics, principally based on the linear approximation, differ in several respects and therefore are still a topic of current discussions. There has been many works using SC method in calculating RTD electronic characteristics and to our knowledge no paper has quantitatively addressed the differences between the two methods in the GaN based RTDs as it will be presented in this work.

The process proposed in this work goes a step further and treat with SC method the calculation of the current density across the device structure under non equilibrium conditions. Indeed, the more quantitative approach would be to consider the external applied field initially in the Hamiltonian system for SC Schrödinger-Poisson simulations and thus for a given bias, the current is determined in a SC manner.

In the present work, we propose to calculate in detail and self-consistently the free electron distribution, the conduction band profiles and the ballistic transport in $Al_xGa_{1-x}N/GaN$ based RTDs at room temperature. For this reason, we have developed a computer code to calculate the electrical properties of $Al_xGa_{1-x}N/GaN$ heterostructures. The electronic subband structures are determined by solving the coupled Schrödinger and Poisson differential equations self consistently via finite differential method [9]. We employ a proper discretization of a non-uniform grid, and taking into account the strong piezoelectric and spontaneous polarization fields exhibited by the wurtzite III-nitride heterostructures. The $J-V$ characteristics are calculated using the transfer matrix formalism assuming a ballistic transport [6]. The effects of the barrier height and internal field on electrical properties of $Al_xGa_{1-x}N/GaN$ RTDs are investigated by varying the Aluminum composition. The influences of crystal layout (*GaN* well width and *AlGaN* barrier thickness) on the current density are also analyzed. A detailed presentation of the employed theoretical model is given in section 2. The results of the band structure and current density calculations are presented in section 3. Finally section 4 concludes the present work.

2. Theoretical formulation

An accurate simulation of resonant tunneling diodes is of primary importance to develop reliable design tools. The RTD structure is treated as an open system and is generally divided into large reservoirs and an active region. The reservoirs model the exchange of electrons with the external electrical circuit. The active region, where the important physical parameters take place, is a short device domain consisting in a single well embedded between two barriers. Thus, numerical calculations should be investigated in such small region. Several items contribute to the high nonlinearity of the device [10] making the simulation of RTDs a delicate assignment.

2.1. Band scheme modeling

To calculate the free-electron distribution and the conduction band profiles we employ the effective-mass approximation. Along the growth direction of the heterostructures (z-axis), the vertical quantum transport requires a SC solution of the coupled one-dimensional Schrodinger and Poisson equations. Within the effective mass theory, the Schrodinger equation is expressed as:

$$\left[-\frac{\hbar^2}{2}\frac{\partial}{\partial z}\frac{1}{m(z)}\frac{\partial}{\partial z}+(eV(z)+\Delta E_c(z)+eV_{xc}(z))\right]\phi(z)=E\phi(z) \tag{1}$$

where $m(z)$ is the position-dependent electron effective mass in the z direction, $V(z)$ is the electrostatic potential and $\Delta E_c(z)$ is a stepwise function due to the conduction band discontinuity. $V_{xc}(z)$ is the local exchange-correlation potential which is discarded in the present investigation because of its minor influence on the results.

The electrostatic potential $V(z)$ *i* s determined by solving Poisson equation in the presence of polarization induced electric field given by:

$$\frac{\partial}{\partial z}\left(-\varepsilon(z)\frac{\partial}{\partial z}V(z)+P_{tot}(z)\right)=q(N_D(z)-n(z)) \tag{2}$$