Transient Quantum Drift-Diffusion Modelling of Resonant Tunneling Heterostructure Nanodevices

Nenad Radulovic, Morten Willatzen, and Roderick V.N. Melnik

Mads Clausen Institute for Product Innovation, University of Southern Denmark, Grundtvigs Alle 150, DK-6400 Sonderborg, Denmark

Abstract. In the present work, double-barrier GaAs/AlGaAs resonant tunneling heterostructure nanodevices are investigated. Numerical results, obtained by in-house developed software, based on a transient quantum drift-diffusion model, are presented and discussed. In the model, quantum effects are incorporated via parameter dependencies on the carrier density gradients. Particular emphasis is given to the carrier densities and quasi-Fermi levels as a function of applied bias, and electrostatic potential profiles inside the resonant tunneling diodes and superlattices.

INTRODUCTION

In what follows, two types of GaAs/AlGaAs resonant tunneling heterostructures are analyzed. The double-barrier resonant tunneling diodes (RTD) with quantum well (QW) width of 2, 5, and 10 nm, barriers and space layers 5 nm each, and contact regions of 26.5, 25, and 22.5 nm, respectively; and the superlattices (SL) made of 2, 3, and 5 QWs, with QWs, barriers and space layers 5 nm each, and contact regions 25 nm. The active regions (QWs, barriers and space layers) are n-type (10^{21} m^{-3}), contact regions are n^+-type (10^{24} m^{-3}), and only the barriers are made of AlGaAs (65% of Al). The bias is applied on the right contact of the nanodevices, while the left contact is grounded. The devices operate at T = 77 K.

THEORY AND NUMERICAL SIMULATION

In the numerical simulation, a transient quantum drift-diffusion model, which is a set of macroscopic semiconductor equations, is employed. The model is originally proposed by Ancona et al. [1], and references therein, and is based on the idea to include density-gradient correction into a generalized transport equation. Hence, the model is powerful enough to account for quantum effects and, at the same time, computationally not very expensive. The model is presented in [2], and a detailed derivation of the model is given in the references therein. The scaled system of three coupled partial differential equations, where the dependent variables are electron density n, quasi-Fermi level F, and electrostatic potential V, is discretized in time and space. The system of nonlinear discretized equations is solved numerically, using matrix form of the Newton iteration procedure.

RESULTS

The maximums of the carrier density, inside the QW of the RTDs (Fig.1), are strongly nonlinear as a function of bias. For small bias, the increase is rapid, and afterwards the maximums reach "saturation" in three orders of magnitude higher region. The increase is monotonous, and only for the RTD with QW = 10 nm, and bias higher than 0.7 V, a light decrease of the maximum value, is observed. In the case of the SL (Fig.2), it is noticeable that the maximums are quite different in different QWs, for the same bias, except for the balance-bias (0.3 V), when the maximums in all QWs reach almost the same value. In the case of RTDs, the maximums of the carrier density for zero bias are strongly different, while in the case of SLs, the maximums are almost the same, for all QWs in all SLs under consideration. In the SLs, the maximums are

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definitely not monotonously increasing functions. The same behavior of the maximums is observed in the case of the SLs with 2 and 3 QWs where the balance-biases are 0.175 V and 0.225 V, respectively. It is common for all SLs that the maximums in the QW close to the grounded contact firstly show a decrease and afterwards reach the highest value for the bias above the balance-bias. The balance-bias has always a value less than the peak-voltage in the N-shape I-V characteristics.

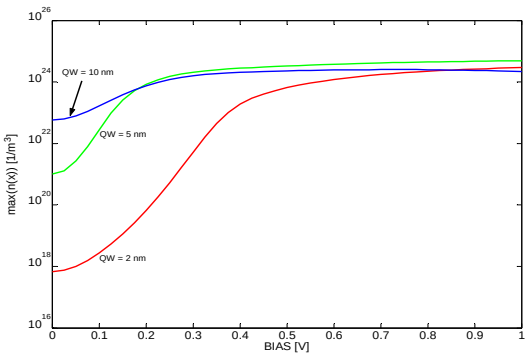

FIGURE 1. The maximums of the carrier density inside the QW of the RTDs as a function of the bias.

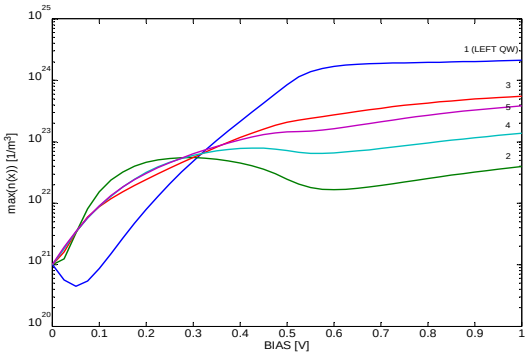

FIGURE 2. The maximums of the carrier density inside the QWs of the SL (with 5 QWs) as a function of the bias.

The quasi-Fermi levels inside the QW of the RTDs (Fig.3), are weakly nonlinear. The same behavior is observed in the case of the quasi-Fermi levels inside the QWs of the SL (Fig.4). In general, the nonlinearity is stronger in the QWs, which are closer to the grounded contact of the SLs. The quasi-Fermi levels in the SLs are not equidistant. The first derivative of the quasi-Fermi levels inside the QWs, as a function of the bias, can indicate the presence and position of the current peak in the N-shape I-V characteristics. Inside the RTDs and the SLs, the quasi-Fermi levels have constant values (in steady state) in the QWs, and in the right contact regions, while in the barriers and in the left contact regions they are definitely not constant.

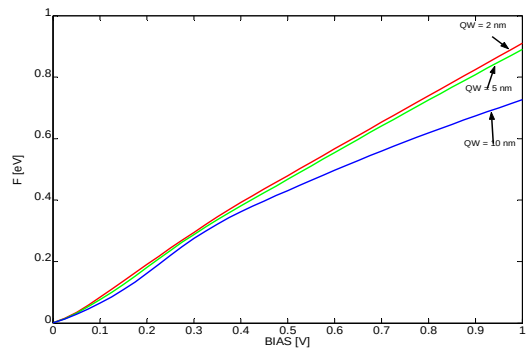

FIGURE 3. The quasi-Fermi levels inside the QW of the RTDs as a function of the bias.

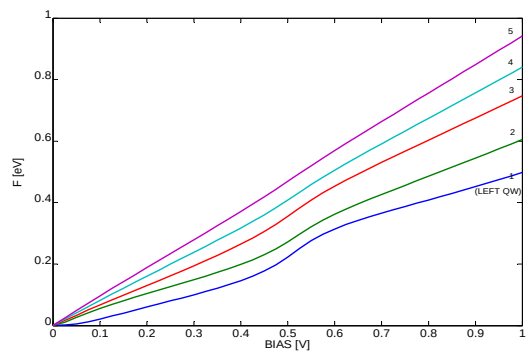

FIGURE 4. The quasi-Fermi levels inside the QWs of the SL (with 5 QWs) as a function of the bias.

The electrostatic potential profiles inside the RTDs and the SLs are nonlinear and the potential drop mainly occurs in the active region (two linear drops with different slopes), and the left contact region (nonlinear drop), while the potential is almost constant in the right contact region (negligible drop).

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