Simulation of Quantum-Ballistic Nanoswitches

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INTRODUCTION

We study quantum-ballistic transport processes in nanoswitches realized by the use of modulation doped heterostructures such as GaAs/AlGaAs layers. These structures have been modelled on the basis of a direct Schrödinger-Poisson approach taking into account also their non-linear behavior.

MODELLING

The electric current through a two-port structure is represented as quantum-ballistic current density

$$J = 2\sum_{t\in T}\int j_{\varepsilon,t}(r)\left(f(\varepsilon,\mu_1)-f(\varepsilon,\mu_2)\right)d\varepsilon \quad (1)$$

This formula is actually the non-linear version of the well-known Landauer-Büttiker formula. Here, it is assumed that the ports are connected - via ideal electron waveguides - with charge reservoirs which are kept in thermodynamic equilibrium. This means that $f(\varepsilon,\mu)$ can be modelled as Fermi-Dirac distribution with μ as the electrochemical potential of the respective contact (Fig. 1).

The wavefunctions in the active area of the device are determined as solutions of the Schrödinger equation in effective-mass formulation

$$\left[-\frac{\hbar^2}{2}\nabla\frac{1}{m^*}\nabla+V_h-e\varphi+V_{xc}[n]-\varepsilon\right]\psi_{j,\varepsilon}=0 \quad (2)$$

with the electrostatic potential φ, the exchange-correlation potential V_{xc} and the step potential of the heterostructure V_h. At the contacts, scattering boundary conditions are assumed. This yields an energy-dependent transmission probability for the scattering states. The resulting wavefunctions are self-consistently coupled to the Poisson equation by the temperature-dependent electron density

$$\rho(r) = \int\sum_j g(\varepsilon)f_j(\varepsilon)\left|\psi_{j,\varepsilon}(r)\right|^2 d\varepsilon \quad (3)$$

The electrostatic potential is calculated using the Green's function method. Practically this approach is equivalent to adding the convolution $G\star\rho$ to the electronic potential without the electrostatic Coulomb potential according to

$$V(r) = V_h(r)+V_{xc}[n](r)-eG(r)\star\rho(r) \quad (4)$$

The assumption that the top surface is metallized leads to the following Green's function:

$$G(r) = \frac{1}{4\pi\varepsilon}\left(\frac{1}{|r|}-\frac{1}{|r-d|}\right) \quad (5)$$

Another modification of the electronic potential originates from the gate-voltages. These will change the number of occupied states of the 2D electron gas at the heterojunction.

RESULTS

The simulations were performed using the 3D simulator SIMNAD [1] and a new non-linear version of the simulator HIGHBIAS [2]. As a first test problem we considered a quantum-wire fabricated and characterized at the University of Würzburg [3]. This structure is built from 40 nm deep and 80 nm wide trenches forming a 100 nm quantum-wire. At a depth of 40 nm underneath the surface a 2D electron gas is easily recognized (Figs. 2, 3).

The influence of the gate voltage is demonstrated by the output characteristics displayed in Fig. 5. We obtain a fairly good agreement betweeen simulation and measurement (Fig. 6) proving the quality of our approach.

ACKNOWLEDGMENT

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REFERENCES

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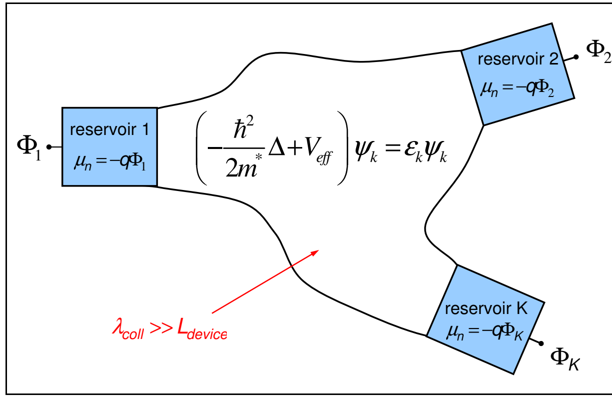

Fig. 1. Basic scheme of simulation domain and boundary conditions (within the active region of the device there are no inelastic scattering processes; only potential-scattering at V_{eff})

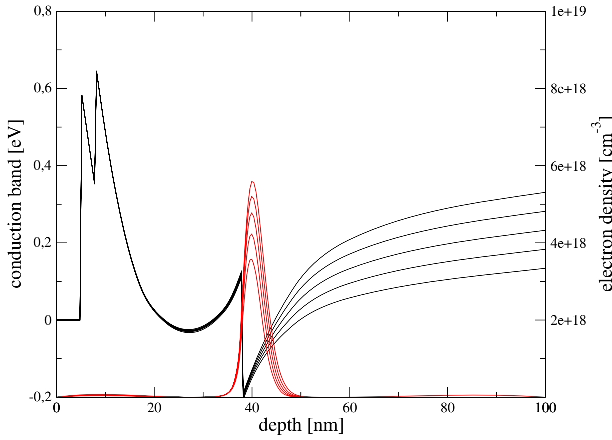

Fig. 2. Conduction band energy and electron density along a vertical cut at different gate voltages (see cut-line in Fig.4)

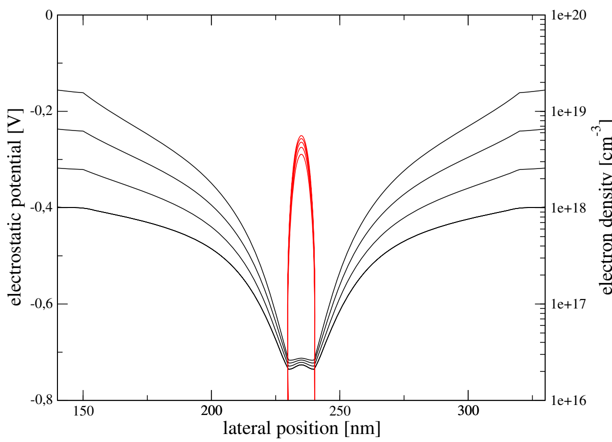

Fig. 3. Electron density and electrostatic potential along a lateral cut at different gate voltages (see cut-line in Fig.4)

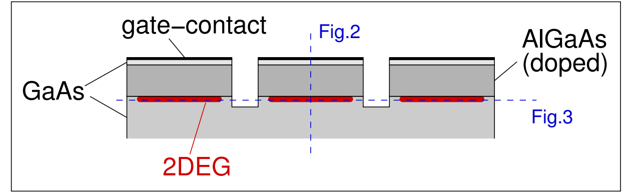

Fig. 4. Schematic view of the trench-controlled 2D quantum-wire structure (lateral cross section)

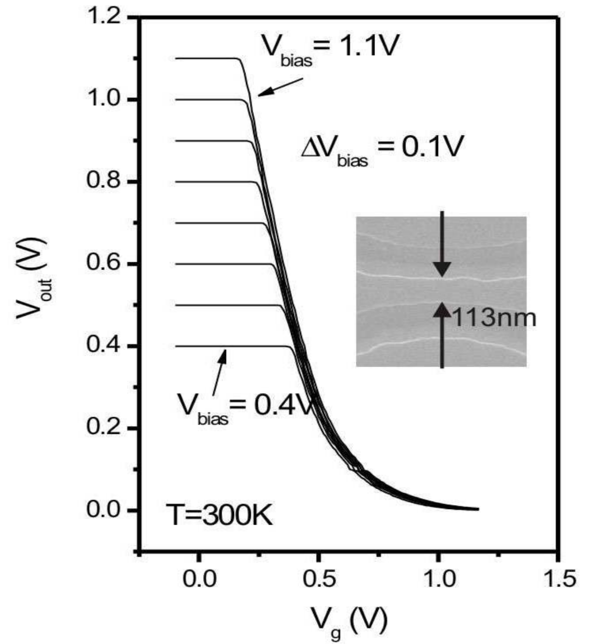

Fig. 5. Measured output characteristics of a quantum-wire structure (obtained from the University of Würzburg) [3]

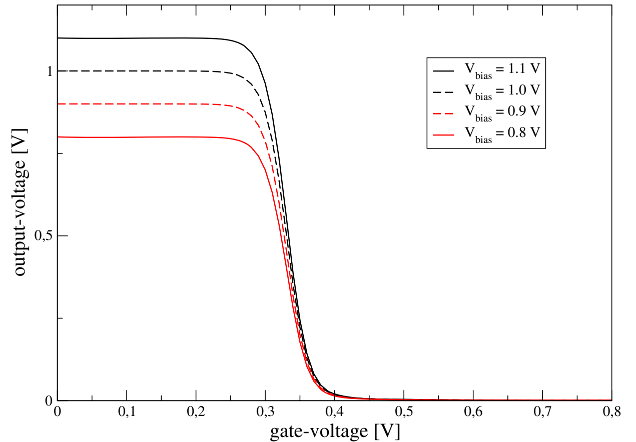

Fig. 6. Simulated output characteristics of a quantum-wire as calculated by SIMNAD