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3D-Simulation of Novel Quantum Wire Transistors

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The output characteristics and the electronic behaviour of a quantum wire transistor (QWT) with a 1DEG channel have been simulated. The electron transport processes in the QWT are mainly influenced by quantum mechanical effects. A coupled microscopic/macroscopic simulation algorithm is used to calculate the electron density distribution in the electron gas under consideration of the confinement of the electrons. This algorithm includes the self-consistent solution of the Poisson and the Schrödinger equation.

Introduction. The structure of the quantum wire transistor (QWT) (Fig. 1) contains a 1D electron gas channel which should be characterised by novel transport properties like ultra high electron mobilities [1]. The atomically precise quantum wire is generated by a MBE technique called cleaved edge overgrowth (CEO) as described in [2]. It involves a regrowth on the sidewall of a cleaved GaAs/AlGaAs heterostructure. Experimental work to this technology and the QWT has been done at the Walter Schottky Institut, TU München.

Several quantum mechanical effects appear with the realization of an 1DEG. The movement of the electrons is confined in one direction. The self-consistent solution of the Poisson and Schrödinger equation is an accurate model to describe the quantum mechanical confinement and to compute the electron density distribution and the discrete electronic states. In the microscopic/macroscopic simulation algorithm the micro-

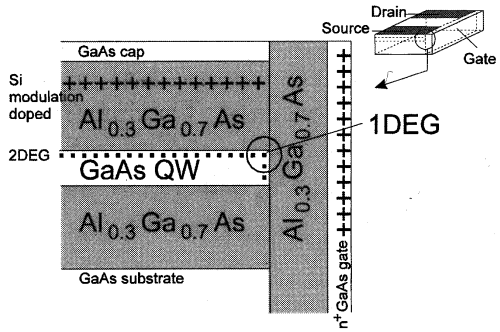

Fig. 1. Quantum wire transistor structure

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scopic model of Schrödinger and Poisson equations is coupled with the known macroscopic drift-diffusion model to compute nanometer devices by using an efficient simulation algorithm.

Model. In the coupled microscopic/macroscopic algorithm [3] the Schrödinger-Poisson solver is used to calculate the electron density distribution and is coupled with the macroscopic transport equations. Because of the 1D confinement of the electrons in the GaAs quantum well near the cleavage plane a 2D solution of the Schrödinger equation is necessary. The Schrödinger equation is solved together with the Poisson equation and coupled with the macroscopic transport equations for the electrons and holes in the area where quantum mechanical effects are expected. In all of the other parts of the device structure the macroscopic drift-diffusion model consisting of the Poisson equation and the transport and continuity equations for the charge carriers is applied.

The solution of the effective mass Schrödinger equation

$$-\frac{\hbar^2}{2}\,\nabla\left(\frac{1}{m^*}\,\nabla\psi\right)+(V-E)\,\psi=0 \tag{1}$$

delivers the discrete energy levels E and the corresponding wavefunctions ψ. The square of the absolute value of the wavefunctions $|\psi_k|^2$ is the occupation probability and n_k is the electron concentration of the energy levels E_k of the quantum wire. The electron density is calculated as [4]

$$n=\sum_k n_k\,|\psi_k|^2+n_{\text{bulk}}\,, \tag{2}$$

$$n_{\text{k, 1DEG}}=\frac{\sqrt{2m^*kT}}{h}\,F_{-1/2}\left(\frac{E_{\text{F}n}-E_k}{kT}\right). \tag{3}$$

The bulk electron density n_{bulk} is assumed in a 3D energy band above the discrete energy levels where the differences between adjoined levels are less than kT.

Algorithm and Numerical Methods. The principle of the coupled microscopic/macroscopic algorithm is described in [3]. The self-consistent solution of the Schrödinger and the Poisson equation delivers the microscopic electron density and the electrostatic potential. After that the charge carrier densities are changed by the solution of the macroscopic transport equations and the next step of the iteration starts. In the transport equations a so-called band parameter is used to simulate heterostructures. This band parameter is influenced by the microscopic solution of the electron density.

The 2D Schrödinger equation is solved at several discretization planes in the direction along the 1DEG. The calculation of the current density in that direction by using the transport equation is possible if the differences between the eigenenergies of adjoining solutions are less than kT.

The solution of the effective mass Schrödinger equation yields to an eigenvalue problem. Dirichlet boundary conditions are used for the Schrödinger equation. Only a limited number of the lowest eigenenergies is required.

For the transformation of the Schrödinger equation into the eigenvalue problem two methods are implemented: the Rayleigh-Ritz method (RRM) [5, 6] and the finite differ-

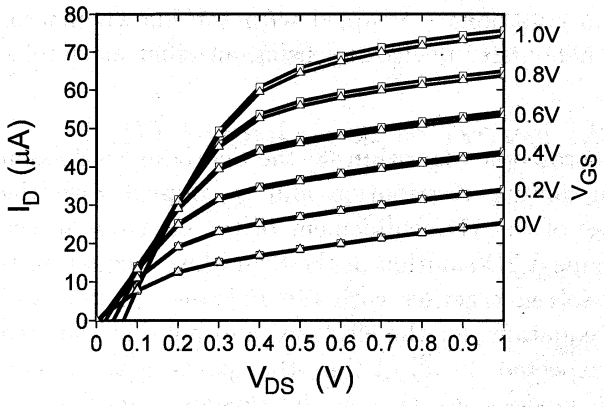

Fig. 2. Output characteristics of the QWT. Triangles: microscopic/macroscopic model, squares: macroscopic model

ences method (FDM) [7]. As an important difference the FDM delivers a symmetric band matrix with a dimension equal to the number of discretization points in contrast to a fully symmetric RRM matrix which dimension is independent of the discretization.

Results and Discussion. The calculated output characteristics of the QWT (Fig. 2) confirm with the typical characteristics of high electron mobility transistors. The results obtained from the coupled microscopic/macroscopic algorithm and from the drift-diffusion model are compared. The microscopic solution shows a smaller drain current because of the more exact used electron density in the 1DEG. This realistic electron density distribution has two maxima at both edges between the AlGaAs layer, the GaAs layer and the sidewall (Fig. 3).

Several variations of the transistor structure regarding the layer thickness and doping and the layout parameters have been analysed. A thinner AlGaAs sidewall causes a higher maximum of the electron density in the 1DEG and consequently higher currents and transconductances appear (Fig. 4). A problem is the increased gate leakage current (see Fig. 2 at small drain to source voltages).

To reduce gate leakage currents the n^+-GaAs gate should not overlap the drain and source regions. The maximum current of such a single QWT is limited by the narrow channel. For an application a channel of a large number of wires should be constructed [1].

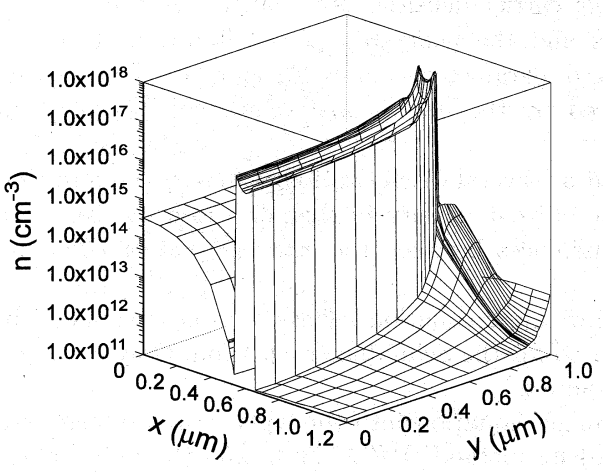

Fig. 3. Electron density of the QWT; $V_{GS} = 1$ V, $V_{DS} = 1$ V

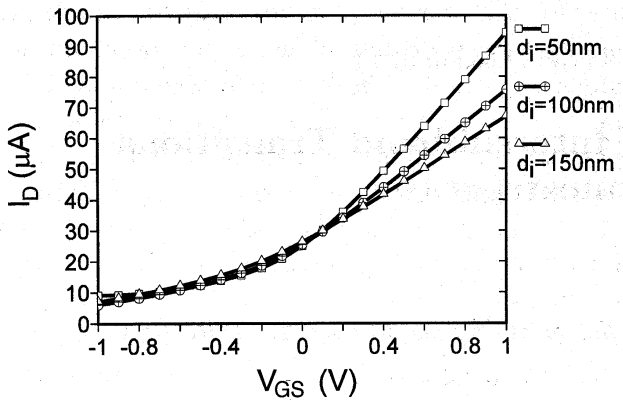

Fig. 4. Transfer characteristics of the QWT; $V_{DS} = 1$ V. Parameter: thickness d_i of the AlGaAs-sidewall

Conclusion. A coupled microscopic/macroscopic simulation algorithm has been used to simulate the electric behaviour of a quantum wire transistor. It includes the self-consistent solution of the 2D Schrödinger and the Poisson equation. An efficient solver for the differential equations and the corresponding eigenvalue problem has been implemented. The simulation results for the QWT with a channel length of 1 μm and at a temperature of 300 K are comparable with the macroscopic solution.

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