Design and Optimization of Complex Nanoscale Electron Devices by Simulations with Quantum Transport Models

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1. Introduction

Integrated circuits which using complex nanoscale electron devices hold promise as a technology for ultra dense high speed integrated digital logic circuits. Especially the negative differential resistance of the current-voltage characteristic in resonant tunneling diodes (RTDs) can be used to reduce device counts per circuit functions, thus increasing circuit integration density. In particular, devices which using RTD structures are attractive for applications in new computing architectures such as neuronal networks and cellular automata, in which even simple functions requires a large number of conventional transistors due to the limited functionality. The advantages of the simulation of nanoscale devices are the fast investigation of different structure variation opposite to a costly manufacturing of semiconductor devices and the better understanding of the inner electron behaviour in nano-structures as well as to find out scaling rules of modern devices with ultra short structure dimensions. For the simulation of complex nanoelectronic semiconductor devices it is necessary that in the physical model quantum mechanical transport phenomena, like tunneling processes of carriers through potential barriers or particle accumulation in quantum wells are included.

2. Simulation models

The simulation models of our device simulator SIMBA are described. The Poisson equation

$$\nabla\left(\varepsilon_s \varepsilon_0 \nabla(\phi)\right) = -q \cdot \left(n - p - N_D + N_A\right), \tag{1}$$

where N_D^+, N_A^- are the ionized donor and acceptor densities, the continuity equations

$$\nabla \cdot \mathbf{J}_n = q \cdot \left(R - G + \frac{\partial n}{\partial t}\right), \qquad \nabla \cdot \mathbf{J}_p = -q \cdot \left(R - G + \frac{\partial p}{\partial t}\right), \tag{2a, b}$$

and the transport equations

$$\mathbf{J}_n = -qn\mu_n \nabla\left(\phi + \lambda_n + \Theta_n\right) + D_n q \nabla(n) + k_B n \mu_n \nabla\left(T_n\right), \tag{3a}$$

$$\mathbf{J}_p = -qp\mu_p\nabla(\phi - \lambda_p - \Theta_p) - D_p q\nabla(p) + k_B p\mu_p\nabla(T_p), \qquad (3b)$$

for the electrons and holes are solved self-consistent in the Gummel algorithm to get the device characteristics at different bias conditions. R and G are the recombination and generation rate, Θ_n and Θ_p are the so-called band parameter for the electrons and holes respectively. In the drift gradient of the transport equations an accessory expression is included, which describes a quantum potential for the carriers

$$\lambda_n = 2\cdot\frac{\gamma_n\hbar^2}{12\,m_n\,q}\cdot\frac{\nabla^2\sqrt{n}}{\sqrt{n}}, \qquad \lambda_p = -2\cdot\frac{\gamma_p\hbar^2}{12\,m_p\,q}\cdot\frac{\nabla^2\sqrt{p}}{\sqrt{p}}. \qquad (4a, b)$$

In the simulation model m_n and m_p are the constant effective mass and the problem of the anisotropic effective mass is handled by the fitting factors γ_n and γ_p. Non-equilibrium device phenomena, like short-channel and overshoot behaviour are taken into account by the energy balance equation and the energy flux density, which is included as additionally equations in the self-consistent Gummel algorithm. The energy flux density equations

$$\mathbf{S}_n = -\kappa_n\nabla(T_n) + \frac{5}{2}\frac{k_B}{q}T_n\cdot\mathbf{J}_n + \frac{3}{2}\lambda_n\cdot\mathbf{J}_n, \qquad \mathbf{S}_p = -\kappa_p\nabla(T_p) - \frac{5}{2}\frac{k_B}{q}T_p\cdot\mathbf{J}_p + \frac{3}{2}\lambda_p\cdot\mathbf{J}_p, \qquad (5a, b)$$

and the energy balance equations

$$\nabla\cdot\mathbf{S}_n = \mathbf{J}_n\cdot\mathbf{E}^* - \frac{3}{2}k_B n\frac{(T_n - T_L)}{\tau_{wn}} - \frac{3}{2}k_B\frac{\partial}{\partial t}(nT_n) - \frac{3}{2}k_B T_n(R-G) + \frac{1}{2}q\lambda_n\left(\frac{n}{\tau_{wn}} - (G-R)\right) + \frac{1}{2}q\frac{\partial}{\partial t}(n\cdot\lambda_n),$$

$$\nabla\cdot\mathbf{S}_p = \mathbf{J}_p\cdot\mathbf{E}^* - \frac{3}{2}k_B p\frac{(T_p - T_L)}{\tau_{wp}} - \frac{3}{2}k_B\frac{\partial}{\partial t}(pT_p) - \frac{3}{2}k_B T_p(R-G) - \frac{1}{2}q\lambda_p\left(\frac{p}{\tau_{wp}} - (G-R)\right) - \frac{1}{2}q\frac{\partial}{\partial t}(p\cdot\lambda_p) \qquad (6a, b)$$

are likewise extended to include quantum effects by the same quantum correction potential for the carriers. τ_{wn} and τ_{wp} are the energy relaxation times. With these quantum hydrodynamic model it is possible to consider quantum mechanical effects, like resonant tunneling of electrons and holes through potential barriers [1]. The Poisson equation (1), the continuity equations (2) and the transport equations (3) without the temperature gradient described quantum drift diffusions processes and denotes as quantum drift diffusion model. Other approaches for the modelling of quantum devices are, for instance, the self-consistent solution of Schrödinger and Poisson equation and the transfer matrix method.

3. Results

3.1 Quantum wire splitting

Fig. 1 shows a 6 nm-$Al_{0.3}Ga_{0.7}As$/GaAs quantum wire structure and the electron density distribution, which is calculated by a quantum drift diffusion transport model. Such structures are used for novel connection concepts as well as for the link up to single electron devices. The feature of the quantum drift diffusion model is the continuity description of the electron density distribution at hetero interfaces in all direction of a complex nanometer structure. The electron density distribution in x-direction is represented in Fig. 2 and compared with a self-consistent solution of Schrödinger and Poisson equation in the vicinity of the quantum well.

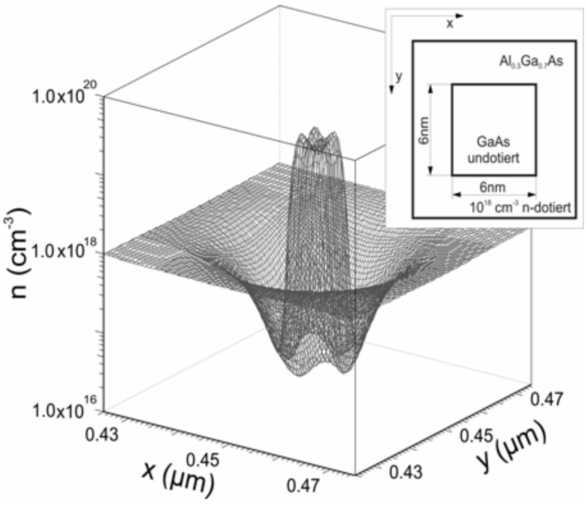

Fig. 1 6 nm-$Al_{0.3}Ga_{0.7}As$/GaAs quantum wire structure and the correspondence electron density distribution

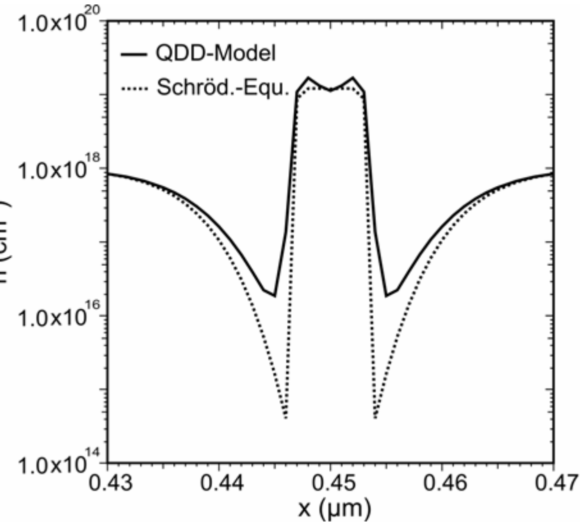

Fig. 2 Electron density distribution in x-direction for different quantum models

3.2 RTDs and monolithic integrated RTD-HEMTs

For the simulation of the different devices (Fig. 3 and Fig. 5) the quantum hydrodynamic transport model is used. Fig 4 shows the current-voltage characteristics of the RTD structure (Fig. 3). The results of the quantum hydrodynamic model are compared with measurement data as well as calculations with the transfer matrix method and show a good agreement.

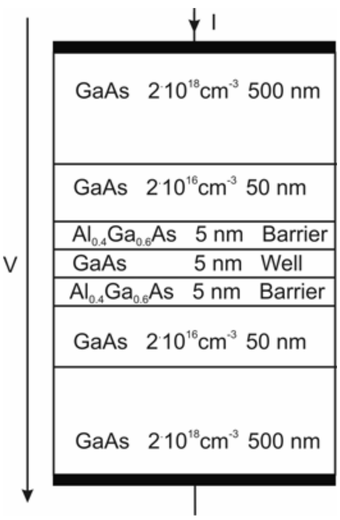

Fig. 3 Structure of the RTD

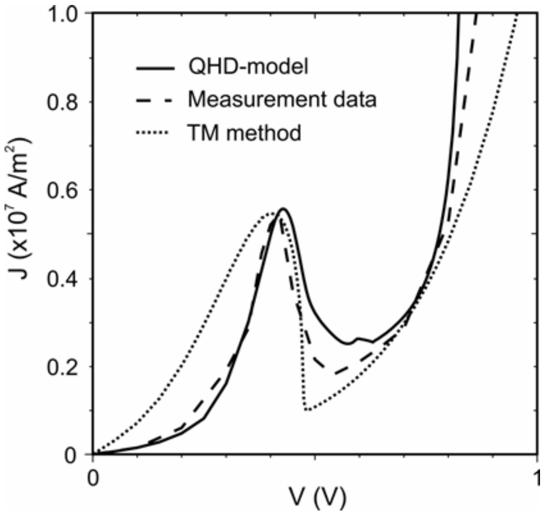

Fig. 4 Current-voltage characteristics of the RTD

The calculated operating principle of a monolithic integrated parallel connection between RTD and HEMT based on $In_{0.53}Ga_{0.47}As$/ $In_{0.52}Al_{0.48}As/InP$ (Fig. 5) is represented in Fig. 6. These kinds of nanoscale devices are applied for high performance monostable bistable transition logic elements, especially for ultra fast logic elements and full adder, which are the main applications for novel nano electronic concepts. The total drain current (I_D) is equal to the sum of the current passing through the RTD (I_{RTD}) and the HEMT (I_{HEMT}). Since the gate-source voltage (V_{GS}) can modulate I_{HEMT}, I_D is also modulated by V_{GS}. The result is that the peak current of the integrated device, especially of the integrated RTD, is modulated by V_{GS}.

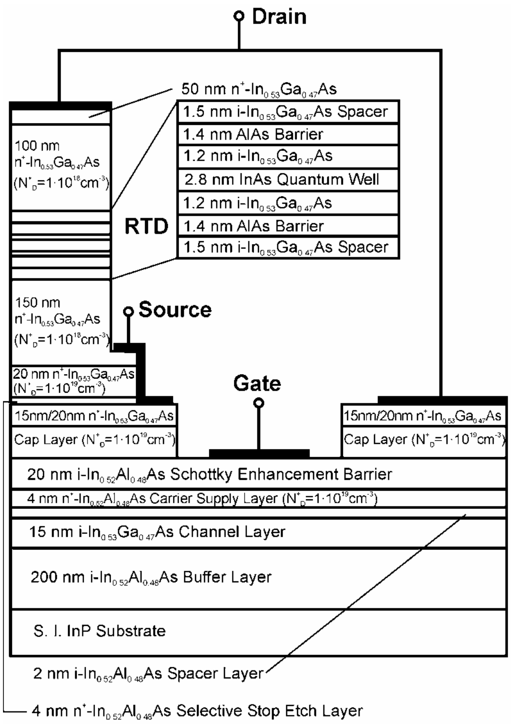

Fig. 5 Schematic cross section of the RTD-HEMT

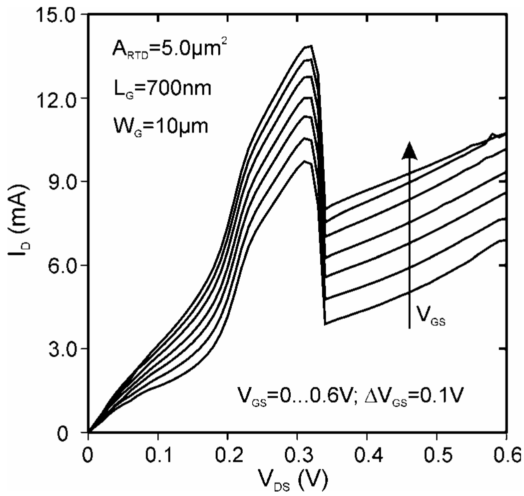

Fig. 6 Output characteristics of the integrated circuit

4. Summary

The quantum drift diffusion and the quantum hydrodynamic models, which are included in our device simulator SIMBA, are described. Numerical 2D-simulations of different nano scale devices, like quantum wires, RTDs and monolithic integrated circuits of RTDs and HEMTs based on $In_{0.53}Ga_{0.47}As/In_{0.52}Al_{0.48}As/InP$ have been carried out.

References

[1] C.L. Gardner: The Quantum Hydrodynamic Model for Semiconductor Devices. SIAM J. Appl. Math., Vol. 54, No 2, pp. 409-427, (1994).