Investigation of Quantum Transport Phenomena in Resonant Tunneling Structures by Simulations with a Novel Quantum Hydrodynamic Transport Model

J. Höntschel, W. Klix, R. Stenzel
University of Applied Sciences Dresden, Department of Electrical Engineering, Friedrich-List-Platz 1, D-01069 Dresden, GERMANY

Abstract This paper describes the simulations of resonant tunneling structures with a novel quantum hydrodynamic transport model. For the simulation the device simulator SIMBA is used, which is capable to handle complex device geometries as well as several physical models represented by certain sets of partial differential equations. As a new feature the involvement of a quantum potential is implemented to include quantum mechanical transport phenomena in different quantum size devices. The coupled solution of this quantum correction potential with a hydrodynamic transport model allows to model resonant tunneling of electrons through potential barriers and particle build up in potential wells. The experimental results of a resonant tunneling structure are compared with the simulated data of the device.

1. Introduction

One intention of modern semiconductor technology is the reduction of the device length and width. With the realization of these nanometer structures several quantum mechanical effects appear. The advancing miniaturizations in the semiconductor technology make it necessary to model quantum effects like resonant tunneling of electrons. The quantum hydrodynamic simulation, which is based of a quantum fluid dynamical model [1], offers expanding possibilities for the understanding as well as the design of novel quantum sized semiconductor devices. The derivation of the full three-dimensional quantum hydrodynamic model (QHD-model), based on the Wigner-Boltzmann equation by a moment expansion, delivers the same conservation laws for the classical hydrodynamic equations, but the energy density and the stress tensor have additional quantum terms. The consequence of these additional quantum terms is the extension of the classical drift diffusion transport equation by an accessory expression, which describes a quantum correction potential. The equation for the energy flux density and the energy balance equation are likewise extended to include quantum effects by the same quantum correction potential. With these quantum terms the resonant tunneling of particles through potential barriers and the accumulation in potential wells can be calculated. The advantage of this model is the macroscopic character, because a description without knowledge of quantum mechanical details like initial wave function is obtained.

2. Simulation model

The Poisson equation

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

(N_D^+, N_A^- ionized donor and acceptor density, ρ_{ADD} additionally fixed charge),
the continuity equations

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

$$\nabla \cdot \mathbf{J}_n = q \cdot \left(R - G + \frac{\partial n}{\partial t} \right), \tag{3}$$

and the transport equations

$$\mathbf{J}_p = -qp\mu_p \nabla(\phi - \lambda_p - \Theta_p) - D_p q \nabla(p) - k_B p \mu_p \nabla(T_p), \tag{4}$$

$$\mathbf{J}_n = -qn\mu_n \nabla(\phi + \lambda_n + \Theta_n) + D_n q \nabla(n) + k_B n \mu_n \nabla(T_n), \tag{5}$$

both for electrons and holes, are solved self-consistently in the Gummel algorithm to get the device characteristics at different bias conditions. R and G are the recombination and generation rate, Θ_p and Θ_n are so called band parameter for holes and electrons respectively, which make it possible to simulate heterostructures. In the drift gradient of the transport equations an accessory expression is included, which describes a quantum potential. Most conveniently the additional force term from the transport equation is personated as the quantum correction potential for electrons and holes

$$\lambda_p = -2 \cdot \frac{\gamma_p \cdot \hbar^2}{12 \cdot m_p \cdot q} \cdot \frac{\nabla^2 \sqrt{p}}{\sqrt{p}}, \tag{6}$$

$$\lambda_n = 2 \cdot \frac{\gamma_n \cdot \hbar^2}{12 \cdot m_n \cdot q} \cdot \frac{\nabla^2 \sqrt{n}}{\sqrt{n}}. \tag{7}$$

For a semiconductor with multiple conduction band minima and anisotropic effective mass the values for m_p and m_n are not clear. In this simulation model m_p and m_n are the constant effective masses and the problem of the anisotropic effective mass is handled by the fitting factors γ_p and γ_n. Non-equilibrium device phenomena, like short-channel and overshoot behavior are taken into account by the energy balance equation and the energy flux density (HD transport model), which are included as additional equations in the self-consistent Gummel-algorithm. The energy flux density equations

$$\mathbf{S}_p = -\kappa_p \cdot \nabla(T_p) - \frac{5}{2} \cdot \frac{k_B}{q} \cdot T_p \cdot \mathbf{J}_p + \frac{3}{2} \cdot \lambda_p \cdot \mathbf{J}_p, \tag{8}$$

$$\mathbf{S}_n = -\kappa_n \cdot \nabla(T_n) + \frac{5}{2} \cdot \frac{k_B}{q} \cdot T_n \cdot \mathbf{J}_n + \frac{3}{2} \cdot \lambda_n \cdot \mathbf{J}_n, \tag{9}$$

and the energy balance equations

$$\nabla \cdot \mathbf{S}_p = \mathbf{J}_p \cdot \mathbf{E}^* - \frac{3}{2} k_B p \frac{(T_p - T_L)}{\tau_{wp}} - \frac{3}{2} k_B \frac{\partial}{\partial t}(pT_p) - \frac{3}{2} k_B T_p (R - G) - \frac{1}{2} q \lambda_p \left(\frac{p}{\tau_{wp}} - (G - R) \right) - \frac{1}{2} q \frac{\partial}{\partial t}(p\lambda_p), \tag{10}$$

$$\nabla \cdot \mathbf{S}_n = \mathbf{J}_n \cdot \mathbf{E}^* - \frac{3}{2} k_B n \frac{(T_n - T_L)}{\tau_{wn}} - \frac{3}{2} k_B \frac{\partial}{\partial t}(nT_n) - \frac{3}{2} k_B T_n (R - G) + \frac{1}{2} q \lambda_n \left(\frac{n}{\tau_{wn}} - (G - R) \right) + \frac{1}{2} q \frac{\partial}{\partial t}(n\lambda_n), \tag{11}$$

are likewise extended to include quantum effects by the same quantum correction potential both for electrons and holes respectively. τ_{wp} and τ_{wn} are the energy relaxations times, which can be calculated by a modified Baccarani-Wordeman model. With these extensions it is possible to consider quantum mechanical effects, like resonant tunneling of electrons and holes through potential barriers and the accumulation of carriers in potential wells.

3. Results

The device structure of the resonant tunneling diode, which was used for the simulation, is represented in Fig. 1 together with the n-type doping densities. This structure was experimentally investigated in [2]. Fig. 2 shows the calculated current-voltage characteristic of a resonant tunneling diode by the QHD-model. Additionally the results of a simulation by a transfer matrix method (TM-method) and measurement data [2] are inserted. The calculated characteristics agree quantitatively at T = 300 K with the experimental values and show a negative differential resistance (NDR). The peak-to-valley current ratio (PVCR) for the QHD-model amounts 2.5, the TM-method results in a PVCR = 5.5 and the experimental results delivers a ratio of 3.0. Fig. 3 illustrates the electron density distribution at different voltages in the range of the NDR and shows charge build up in the quantum well. The electron temperature for the same voltages is represented in Fig. 4. A high electron temperature behind the barriers can be detected. In this range a strong increase of the temperature gradient can be indicated, which is included in the transport equations.

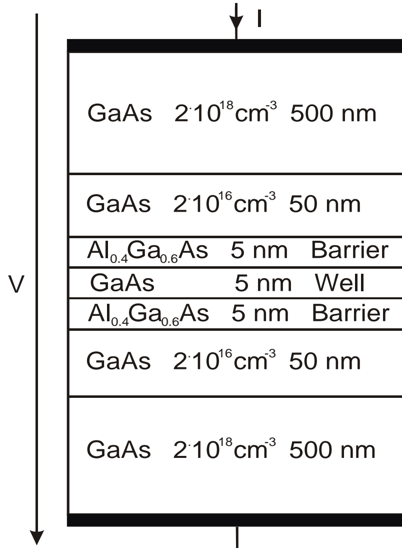

Figure 1 Structure of the RTD

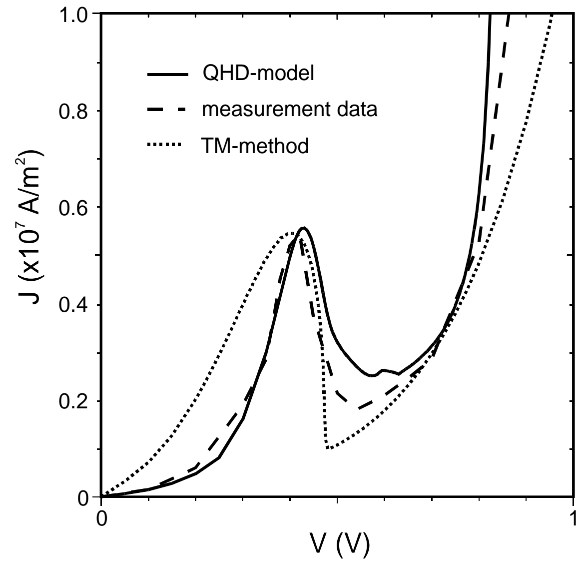

Figure 2 Current-voltage characteristics

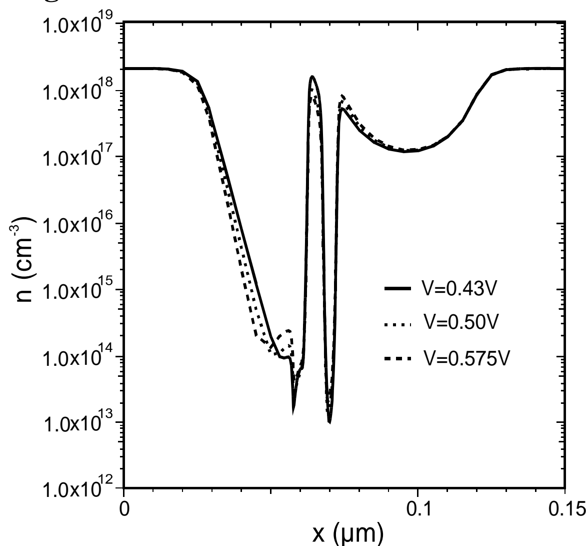

Figure 3 Electron density distribution

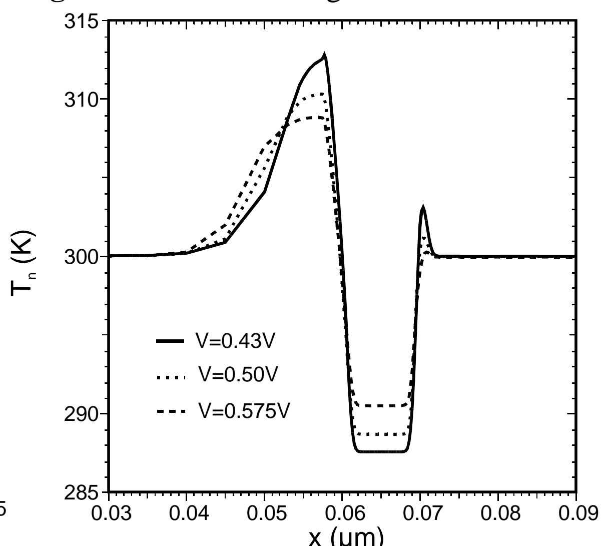

Figure 4 Electron temperature

Further investigations of some structure modifications have been carried out. Especially the thickness of the quantum well is varied between l_w = 3 nm to l_w = 7 nm. Fig. 5 shows the dependence of the first sub-band energy and the separation to the second sub-band

energy on the thickness of the quantum well in the thermal equilibrium, which is calculated by a self-consistent solution of Schrödinger and Poisson equation. With a decrease of thickness an increase of the first sub band energy and a stronger separation to the second sub band energy occurs. This behavior results in a shift of the tunneling maximum to higher bias voltages and larger PVCRs. Fig. 6 illustrates the simulated current-voltage characteristics of a parallel connection of 3 RTDs with different thickness ($l_w = 3$ nm, $l_w = 4$ nm and $l_w = 7$ nm). Additionally the separated current-voltage characteristics of the three different RTDs and the sum of these characteristics are inserted. A good agreement between the local maximums of the separated characteristics and whose simulated results of the parallel connection can be detected. The differences between the sum of the characteristics and the simulated data of the real calculated quantum size device results from the corners at the interface of the different RTDs with varied thickness of the quantum well.

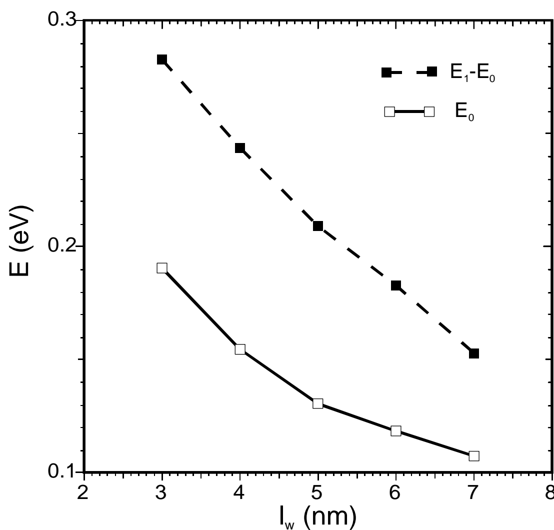

Figure 5 First sub band energy and separation to the second sub band energy as a function of the quantum well thickness

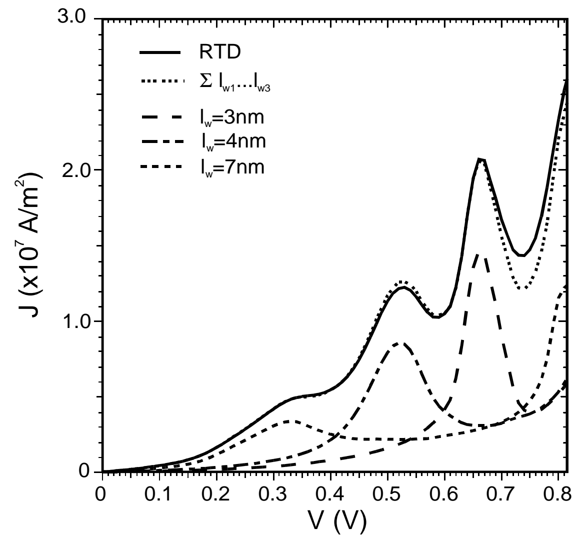

Figure 6 Current-voltage characteristics for a parallel connection of 3 RTDs with different quantum well thickness

4. Conclusions

Numerical 2D-simulations with a novel quantum hydrodynamic transport model of resonant tunneling structures have been carried out. For the calculations, a solution of a quantum correction potential is used, which is included in the hydrodynamic transport model. The simulated RTD structure shows a good agreement with measurement data. The structure variations exhibit a shift of the tunneling maximum to higher bias voltages at a decrease of the quantum well thickness. With the novel quantum hydrodynamic model it is possible to take into account quantum mechanical effects in all directions of a complex nanometer structure.

References

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

[2] A.M.P.J. Hendriks, W. Magnus, and T.G. van de Roer: Accurate Modeling of the Accumulation Region of a Double Barrier Resonant Tunneling Diode. Solid-State Electronics, 39, pp. 703-712, (1996).