Efficient quantum-mechanical model based on drift-diffusion approach for simulations of modern nanoscale devices

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Abstract

A simple and efficient quantum-mechanical model for simulation of modern nanoscale devices is presented. The model was used for quantitative calculations of quantum currents in nanoscale electronic devices. Specifically, we used it to simulate the tunnelling current in the test structure, direct and reverse tunnel currents through the tunnel junction, Schottky contact, etc. The model has been implemented successfully within the drift-diffusion approach of our NanoTCAD simulator. We provided a series of simulations and compared them with published data, experimental measurements and other complicated models, including the Wigner function method, quantum Boltzmann transport models, and others.

Keywords: Simulations; Nanoscale devices; Drift-diffusion; Tunnelling

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1. Introduction

The progress in large-scale integration (LSI) technologies has resulted in scaling down semiconductor devices to nanoscale dimensions where kinetic and quantum effects in the carrier transport become crucial for the device performance. Designing an efficient simulation tool for such devices involves a trade-off between the efficiency and accuracy.

Drift-diffusion (DD)-based models have a long and fruitful history in applications to simulations of not only modern electronic devices [1,2] but also optoelectronic devices [3]. In recent years, however, a new class of devices has emerged requiring tools that include quantum effects and also allow for efficient numerical implementation. One such device is the vertical cavity surface-emitting laser (VCSEL) with tunnelling injection (TI) [4,5]. For the efficient simulation of such devices, we have developed a new and efficient model.

The model summarized here has been implemented successfully within the drift-diffusion approach of our NanoTCAD simulator [6]. We provided a series of simulations and compared them with published data, experimental measurements and other complicated models, including the Wigner function method, quantum Boltzmann transport models, and others. For more details, see Fedoseyev et al. [7] and our recent review [8].

2. Drift-diffusion with quantum corrections

Our model is based on DD with the added quantum corrections in the appropriate areas. The brief description is as follows. The formula for the tunnelling current between two bulk regions with parabolic energy bands (which includes the potential bias V through the barrier) can be written as [3]:

$$J_{tun} = \frac{qm^* k_B T}{2\pi^2\hbar^3} \int_{E_{\min}}^{E_{\max}} dE_z T(E_z) \times \ln\left\{ \frac{1 + \exp\left[-(E_z - V - E_{Fn,left})\right] / k_B T}{1 + \exp\left[-(E_z - E_{Fn,right})\right] / k_B T} \right\} \quad (1)$$

where E_z is the energy of motion perpendicular to the tunnel junction (a similar expression holds for holes). Note that the tunnel current vanishes for $V = 0$ and $E_{Fn,left} = E_{Fn,right}$.

For a description of transport problems with potential barriers, one can try the DD approach. It is known, however, that the DD model gives a low current if a

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potential barrier is created in a simulated device (by a factor of two to three). One of the ways to improve the accuracy of the DD model in such a case is to take into account the tunnelling current through the barrier region. In the NanoTCAD simulator [6], we implemented an analytical formula for the tunnelling current in a rectangular barrier.

3. Tunnelling mobility

The important question in practical development is how to incorporate the tunnelling current as described by Eq. (1) for a particular device structure into the code. We proposed to do this via the 'tunnelling mobility'. This surprisingly simple trick works very well, and the modifications of NanoTCAD simulator code are minimal and very localized.

Tunnelling mobility is implemented in the following way. We assume that the tunnelling current is proportional to tunnelling mobility within the quantum well (QW)

$$J_T = \mu_T E n_n \tag{2}$$

and the current J_T is calculated by Eq. (1). Thus, the tunnelling mobility is defined by the following equation:

$$\mu_T = \frac{J_T}{n_n(x)E} \tag{3}$$

The electric field E in the quantum well is approximated as

$$E = V/d \tag{4}$$

where V is the electrostatic potential difference (bias) at the QW and d is the QW thickness. The DD model is used in the rest of the device in the NanoTCAD simulator.

4. Results and conclusions

Our main conclusions are that the proposed model is quite accurate and computationally efficient. The results for a single barrier device show a good agreement with Wigner function method results (Fig. 1). The Schottky contact model compares well with experimental measurements. The tunnel junction model has correctly demonstrated negative differential resistance for forward bias and exponentially growing current for the reverse bias. The implementation is self-consistent, has no tune-up parameters, and has not caused slow convergence or numerical instability in the validation test presented.

Experimental data for a single barrier device would be the best test case, but they are not available. Instead, we chose the single tunnelling barrier test problem. This

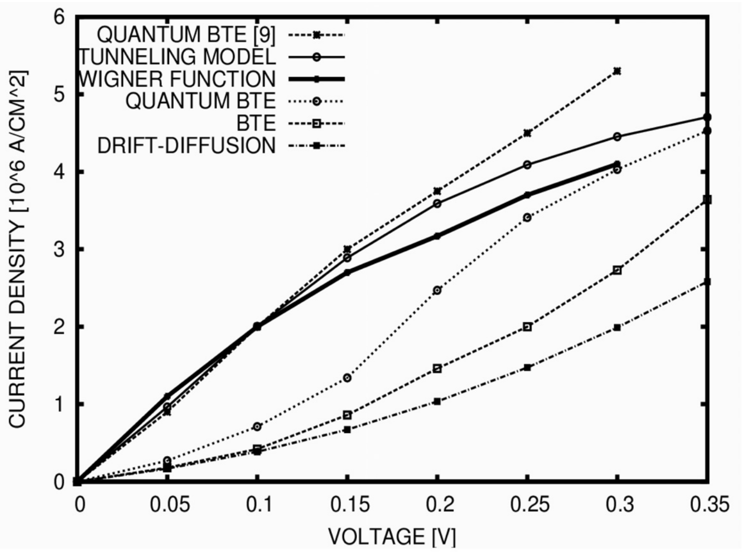

Fig. 1. Results for the test problem ($T = 300\,\mathrm{K}$, doping density $10^{18}\,\mathrm{cm}^{-3}$, bias up to 0.35 V). IV curves (from upper to lower): 1, quantum BTE [9]; 2, NanoTCAD simulator DD with tunnelling model; 3, Wigner function method [9]; 4, quantum BTE (NanoTCAD simulator); 5, BTE (NanoTCAD simulator, [9]); 6, DD results from NanoTCAD simulator. The BTE solutions with NanoTCAD simulator compare well with one from ref. [9]. The NanoTCAD simulator DD with tunnelling model compares well with Wigner function method results (even better than quantum Boltzmann solutions).

problem has been solved by different methods and independently by different authors. The test structure consists of a 2.5-nm 0.22 V AlGaAs barrier in a 40-nm GaAs/AlGaAs device. This problem was solved by using (i) the Wigner function method [9], (ii) the quantum Boltzmann transport equation [7,9] (iii) the Boltzmann transport equation [7,9] and (iv) the DD model [7]. The results are shown in Figs. 2, 3 and 4. More details on this are available [7–9].

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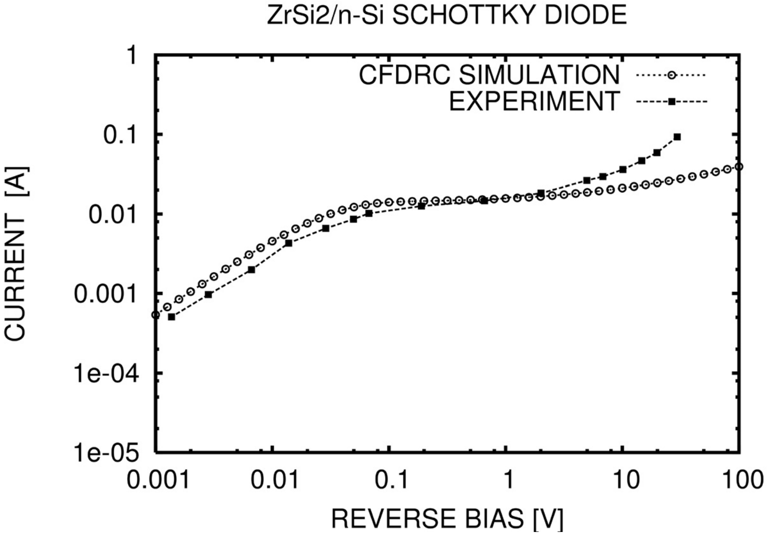

Fig. 2. Comparison of numerical (NanoTCAD simulator) and experimental [10] IV curves for low-doping Schottky diode, $ZrSi_2$/n-Si $j_b = 0.55\,V$, $N_d = 3.510^{15}\,cm^{-3}$.

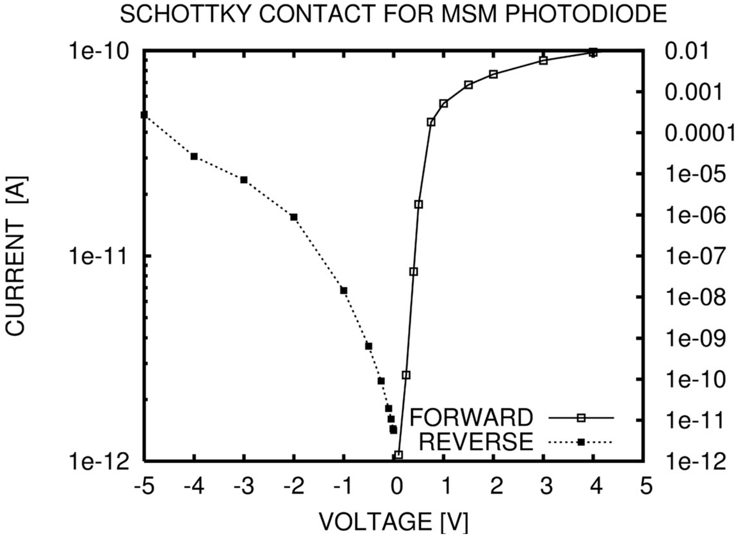

Fig. 3. Results of NanoTCAD simulator modelling for Philips MSM photodetector [11]: IV curve for reverse and forward biases.

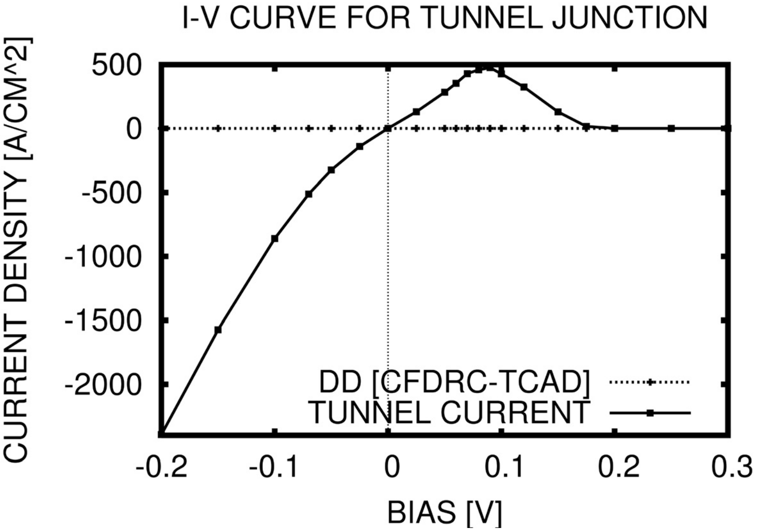

Fig. 4. New quantum model for a tunnel p-n junction (used in VCSEL): IV characteristics. Both NDR and exponential growth at reverse bias are reproduced well.

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