Robust Computational Models of Quantum Transport in Electronic Devices

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A family of efficient quantum transport models for simulation of modern nanoscale devices is presented. These models are used for quantitative calculations of quantum currents in nanoscale electronic device within our device simulator software. Specifically, we used them to simulate the tunneling current through thin barrier in VCSEL, direct and reverse tunnel currents through the tunnel junction, Schottky contact, gate induced drain leakage (GIDL), etc.

The models have been successfully implemented within the drift-diffusion approach of CFDRC-TCAD simulator. In particular, to take into account the tunneling current through the thin potential barrier, we introduced the concept of " tunnel mobility" For the Schottky contact problem, in cases when quantum effects dominate, we have used a series of analytical approximations for different ranges of temperature, doping, and voltage.

We performed a series of simulations to compare these fast and efficient models with published data, experimental measurements, and other sophisticated models, including Wigner function method, quantum Boltzmann transport models, and others [1-5].

We can conclude that: the proposed models are quite accurate, and computationally efficient. The results for single barrier device show a good comparison with Wigner function method results for the *2.5 nm 0.22V AlGaAs* barrier in *40 nm GaAs/AlGaAs* device (Fig. 1). This problem was solved also with Quantum Boltzmann transport equation, Boltzmann transport equation [1], and the drift-diffusion model. Our " tunneling mobility" model for DD method compares well with Wigner function method results. Our Schottky contact model results compared well with experimental measurements [4,5] (Fig.2, 3). Tunnel junction model has correctly demonstrated negative differential resistance for forward bias and exponentially growing current for the reverse bias (Fig. 4).

The proposed implementations are self-consistent, has no tune-up parameters, and have not caused slow convergence or numerical instability in the validation tests performed.

REFERENCES

1. A. Fedoseyev, V. Kolobov, R. Arslanbekov and A. Przekwas, (2003), Kinetic simulation tools for nanoscale semiconductor devices, *Microelectronic Engineering*, v. **69** (2003) p. 577-586.
2. Tsuchiya, H. and T. Miyoshi, (1999) Quantum Transport Modeling of Ultrasmall Semiconductor Devices, *Special Issue on TCAD for Semiconductor Industries. IEICE Trans. Electron* E82-C, 880.
3. Ja-Hao Chen, Shyh-Chyi Wong, and Yeong-Her Wang (2001), An Analytic Three-Terminal Band-to-Band Tunneling Model on GIDL in MOSFET, *IEEE Trans. Electron Devices,* **48**, 2001 , 1400.
4. J. M. Andrews and M. P.Lepselter (1970), Reverse current-voltage characteristics of metal-silicide Schottky diodes, *Solid-State Electron.*, **13**, 1970, 1011.
5. M. Seto, J.-V. Ledue and A.M.F. Lammers (1997), Al-n-Si Double-Schottky Photodiodes for Optical Storage Systems, ESSDERC 97, Stuttgart, 22-24 September 1997

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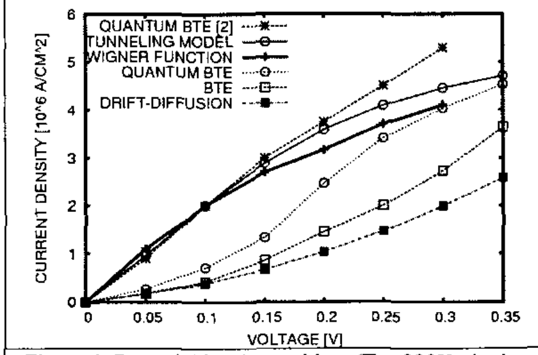


Figure 1. Potential barrier problem (T = 300K, doping 10^{18} cm^{-3}), IV curves (from top to bottom): 1 - quantum BTE [2], 2 – (CFDRC-TCAD solver, DD with tunneling model, 3 - Wigner function method [2], 4- Quantum BTE (CFDRC), 5- BTE (CFDRC and [2]), 6-DD results from CFDRC-TCAD solver [1].

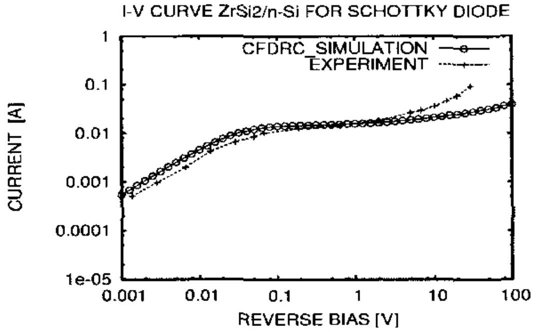
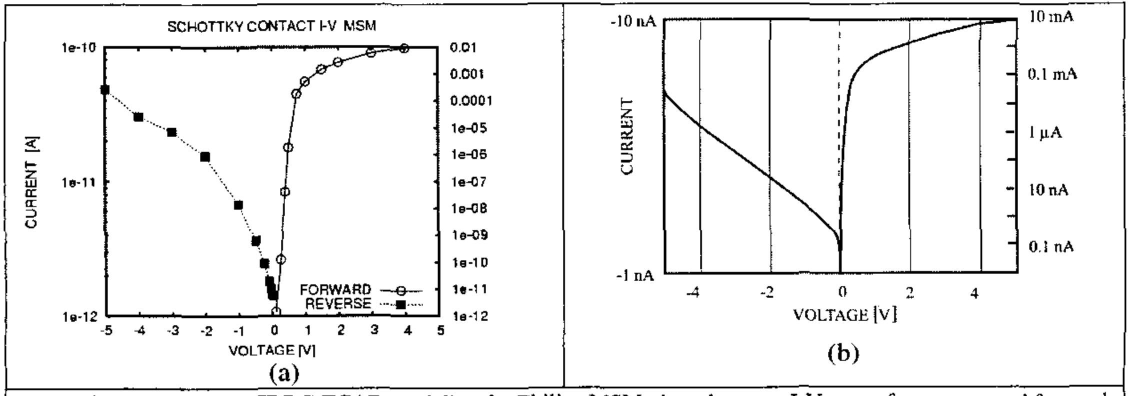


Figure 2. Comparison of numerical (CFDRC-TCAD) and experimental [4] I-V curves for low-doping Schottky diode, ZrSi2/n-Si, ψ_b=0.55V, N_d=3.5 10^{15} cm^{-3}



(a)

(b)

Figure 3 (a) Results of CFDRC-TCAD modeling for Philips MSM photodetector: I-V curve for reverse and forward biases. and experimental data; (b)Philips MSM photodetector experimental data for reverse and forward biases [5].

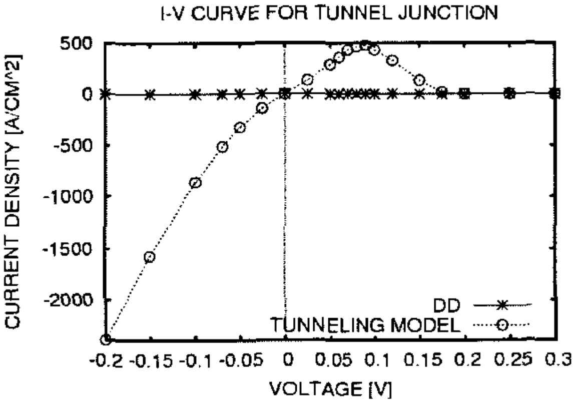


Figure 4. New quantum model for a tunnel p-n junction (used in simulation of VCSEL): I-V characteristics. Both negative differential resistance (NDR) and exponential growth at reverse bias are reproduced well with this model. For comparison, the DD model result is shown; its current is nearly zero for this bias range.

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