Modeling Transients in Nanostructures

B. Novakovic and I. Knezevic
Department of Electrical and Computer Engineering, University of Wisconsin-Madison
1415 Engineering Drive, Madison, WI 53706, USA
e-mail: novakovic@wisc.edu

INTRODUCTION AND MOTIVATION

Modeling electronic devices in the transient regime is a topic of great interest in designing analog and digital electronic circuits. It allows optimizations of devices with respect to achieving high switching and cut-off frequencies. Specifically, efficient sources, mixers, and other functional blocks in the terahertz frequency window (300 GHz – 3 THz) have important applications in chemical and biological sensing, medical imaging, astronomy and communications. A possible path toward achieving efficient electronic circuitry in the terahertz window is increasing the frequency at which solid-state electronic devices can amplify and oscillate.

In this paper, we develop the theory and computational methods for modeling the transient regime in two-terminal ballistic nanostructures connected with dissipative macroscopic contacts. The question we want to answer is how the current, as well as the potential and charge density, evolve in time in response to a sudden change in bias. The ballistic nanostructure assumption is meaningful, since the dephasing length in the contacts is of the same order of magnitude as the size of contemporary circuits (~50 nm for heavily doped Si at T = 300 K).[1] The two-terminal set-up is an important case, having in mind that the fastest devices today are Schottky and resonant tunneling diodes (RTDs), with RTDs already being able to oscillate above 1 THz frequencies.[2] This is largely due to diodes being much less affected by parasitic capacitances that are intrinsic to complex transistor layouts.

THEORY

Our approach is based on the density matrix theory in the open system formalism. The model nanostructures we consider are represented through the density matrix which evolves in time through the interaction of the nanostructure with its environment. Assuming that the initial density matrix of the total system is separable (not entangled) $\rho_{tot} = \rho_C \otimes \rho_S$, where ρ_C and ρ_S are the contact and nanostructure (S stands for "system") density matrices, respectively, we have

$$\frac{d}{dt}\rho_S(t) = F(t)\rho_S(t). \qquad (1)$$

Equation (1) describes the subdynamics of the nanostructure, where $F(t)$ is the time evolution operator. The time evolution operator can be conveniently derived in the case of relevance: that of the relaxation time in the contacts (τ = 10 - 100 fs) being much shorter than the total relaxation time (τ_S = 10 – 1000 ps). The solution to Eq. (1) gives the time evolution of the nanostructure distribution functions.[3,4] When coupled with the solution to the time-independent Schrödinger equation, with the Hartree potential included, Eq. (1) leads to a complete model for calculating the time dependence of the current, as well as charge density and potential inside the nanostructure.

SIMULATION

The computational algorithm consists of coupling the equation which is the solution to Eq. (1), the time-independent Schrödinger equation, and the Poisson equation, in both 1D and 2D applications. Real-space modeling is implemented by using the central finite-difference and finite element methods (in 1D and 2D, respectively),[5] while the time dependence is computed using the backward finite-difference. The resolution in space (~0.5 nm) was chosen to allow sufficiently dense discretization of the continuous energy

spectrum of the model nanostructure, while the resolution in time is no greater than τ.

RESULTS

Figures 2 and 3 show sample results of the computation for the case of 2D narrow quantum point contact (QPC), shown in Fig. 1. The results are representative of the range of modeled nanostructures in 1D and 2D: the time evolution of the nanostructure is dependent on its transmission properties and the scattering mechanisms in the contacts. Specifically, as long as $\tau << \tau_S$, contacts with longer relaxation time τ allow shorter time to steady state, as shown in Fig. 3. The red curve in Fig. 3 is on the edge of the allowed region ($\tau << \tau_S$), but it helps to visualize the general trend.

ACKNOWLEDGEMENT

This work has been supported by the NSF (award ECCS-0547415).

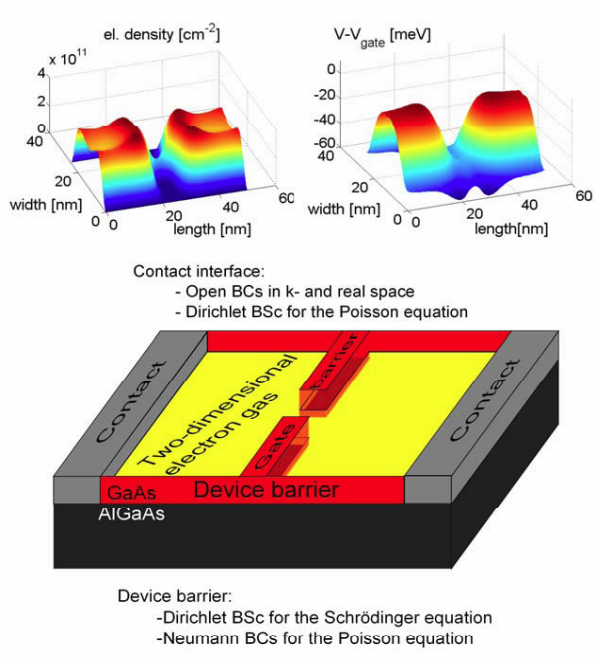

Fig. 1. The narrow QPC structure schematic, with different regions and associated boundary conditions (lower panel), and the charge density and potential in equilibrium (upper panel). The sheet density is 2.3 x 10^{11} cm^{-2}, T = 77 K, and the momentum relaxation time is $\tau \approx 140$ fs.

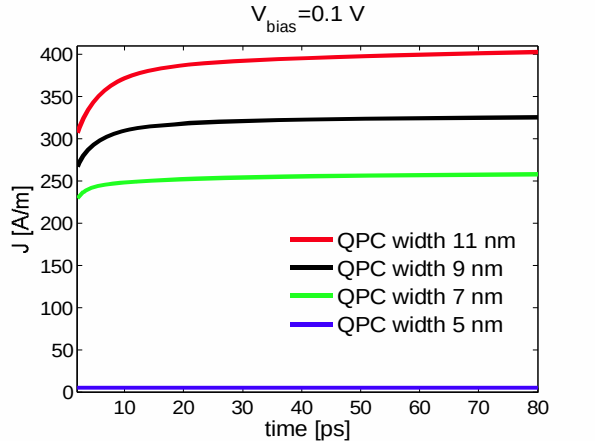

Fig. 2. Dependence of the transient current density on the QPC width.

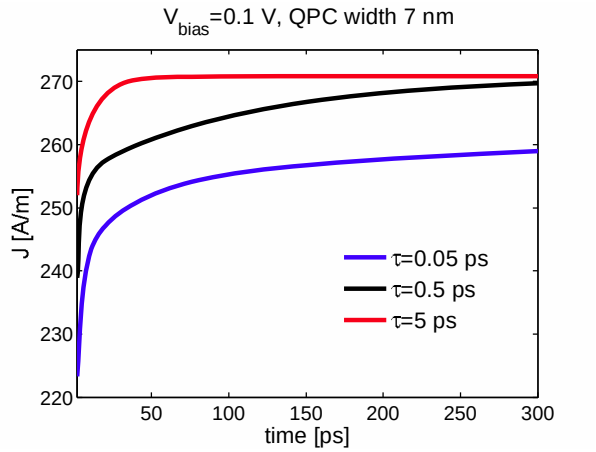

Fig. 3. Dependence of the transient current density on the relaxation time in the contacts.

REFERENCES

[1] M. V. Fischetti, *Master-equation approach to the study of electronic transport in small semiconductor devices*, Physical Review B **59**, 4901 (1999).

[2] M. Feiginov, C. Sydlo, O. Cojocari, and P. Meissner, *Resonant-tunnelling-diode oscillators operating at frequencies above 1.1 THz*, Applied Physics Letters **99**, 233506 (2011).

[3] I. Knezevic, *Decoherence due to contacts in ballistic nanostructures*, Physical Review B **77**, 125301 (2008).

[4] B. Novakovic and I. Knezevic, *Quantum master equations in electronic transport*, in *Nano-Electronic Devices: Semiclassical and Quantum Transport Modeling*, D. Vasileska and S. M. Goodnick, Eds., New York: Springer, 2011, ch. 4, pp. 249-287.

[5] S. E. Laux, A. Kumar, and M. V. Fischetti, *Analysis of quantum ballistic electron transport in ultrasmall silicon devices including space-charge and geometric effects*, Journal of Applied Physics **95**, 5545 (2004).