

# Advanced Device Simulation and Modeling

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#### **Abstract**

This poster gives a short overview on advanced semiconductor simulation and modeling related issues and motivates the extension of classical numerical device simulators. Three examples show schematically where shrinking dimensions lead to non-classical effects.

### Introduction

Device simulation tools are designed to assist in technology developement and compact modeling since device simulation provides insight into the behavior of semiconductor devices by means of the distribution of internal device quantities, instead of global quantities such as current-voltage characteristics alone. Therefore, device simulations tools should allow to include all relevant effects describing the device behaviour fairly accurately.

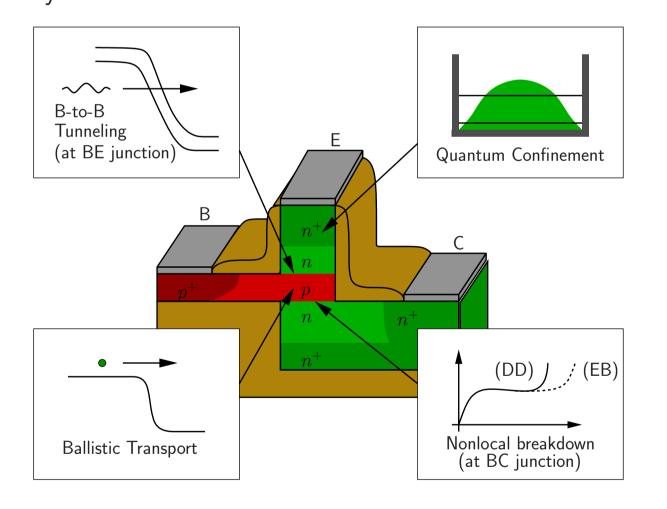


Figure 1: Non-classical effects in THz HBTs. (Semiconductor heterostructure technology is used for highest-performance electronic technologies developed today. The advantage of heterostructures is that they provide a means to control the motion of carriers over nanoscale dimensions. This technological control can be exploited in many ways to improve device performance. For example, a heterojunction can encourage the transport of electrons while suppressing the transport of holes; this effect is exploited in heterojunction bipolar transistors (HBTs). With ongoing downscaling of the dimensions, the behavior of the device is affected significantly by means of non-classical effects. A drastically reduced base width decreases the probability of carrier scattering leading to quasi-ballistic carrier transport with improvements in carrier velocity and time constants. Further shrinking of the emitter width cause quantum confinement and hence modified capacitances and current paths.)

With the ongoing shrinking of the physical dimensions of semiconductor devices and emerging new device concepts using directly quantum effects for operation, various shortcomings of classical device simulators appear. These tools are frequently based on semi-classical drift-diffusion transport model and fail

to predict the behavior of advanced devices due to the lack of quantum mechanical physics and proper description of non-local effects. Non-classical effects comprises quantum as well as non-local effects. Some of them are motivated below. Three examples shows schematically where these non-classical effects are expected with shrinking device dimensions.

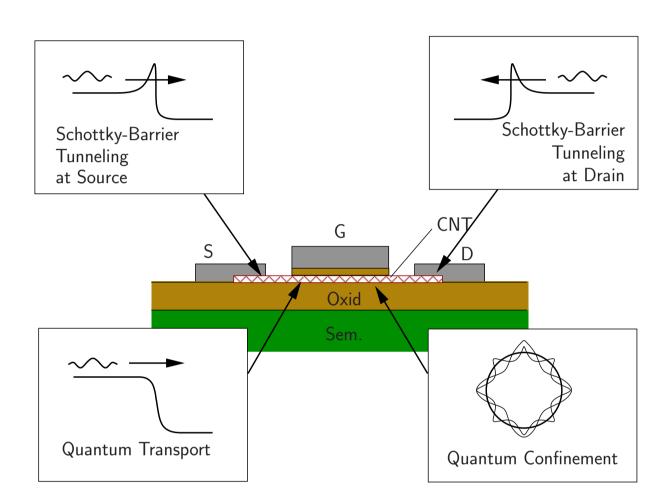


Figure 2: Quantum effects in carbon nanotube transistors. (Further downscaling of conventional MOS transistors into the sub 10nm range is eventually limited by physical and technology constraints. Hence, developing conceptually new devices exploiting quantum effects rather then suffering from them is becoming increasingly important. New nanoelectronic devices, such as carbon nanotubes (CNT) transistors considered to be the most prominent candidates for the post CMOS era. New nanoelectronic devices are expected to complement and substitute some of the current cmos functions after being integrated into cmos technology. The operation of CNT transistors inherently bases on quantum mechanical effects.)

# Non-local effects

Shrinking dimensions increase the local electric field leading to an energy imbalance between carriers and lattice. This imbalance influences the device behavior and, hence, several device characteristics. Changes in device characteristics due to energy imbalance are often called *non-local effects* since the energy of a carrier depends on its covered path. These non-local effects influences, e.g., the breakdown voltage and the charge storage in HBTs (see Fig. 1). Device simulations should include models to take into account the carrier energy separately by solving the energy balance equation self-consistently with the classical drift-diffusion model.

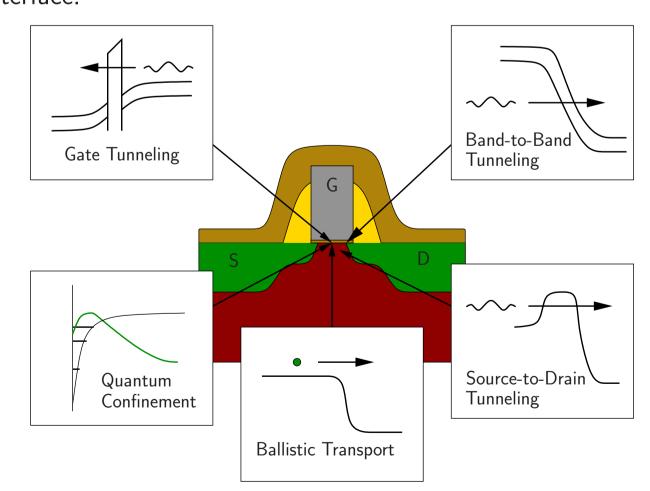
Reduced length of carrier transport path also drastically decreases the probability of carrier scattering. Almost scattering free transport is called *quasi-ballistic* transport [1, 2] which significantly influences, e.g., the carrier velocity and time constants (see Fig. 3). Depending on the transport path length, quasi-ballistic transport is accurately described with a semi-classical approach or with a quantum approach. To include quasi-ballistic

quantum transport, the Schrödinger equation and the Landauer equation should be solved self-consistently with the Poisson equation.

#### **Quantum Confinement**

If the dimension of potential wells in conduction or valence band edge reaches the de Broglie wave lengths of the carries, the energy within the bands is rather quantized than continuous. Carriers confined within potential wells can only have one of these quantized (discrete) energies  $E_n$ . The square magnitude  $|\psi_n|^2$  of the wavefunction  $\psi_n$  of an confined electron equals the probability to find the electron with energy  $E_n$  at a certain position within the potential well. The quantized energies  $E_n$  and the wavefunctions  $\psi_n$  can be obtained with a self-consistent solution of the Schrödinger and the Poisson equation with appropriate chosen boundary conditions [3]. It is common to use the time-independent effective mass Schrödinger equation.

Quantum confinement significantly changes the electron concentration within a quantum well. Generally, the peak of electron concentration is shifted from the potential barriers into the center of quantum well. This effect has significant influence, e.g., on the electron concentration in the channel of MOS transistors (see Fig. 3) and in the quantum well perpendicular to heterojunctions. Further, since the electron concentration is shifted away from interfaces between different materials, the scattering rates due to interface scattering are significantly reduced since the current flows some nanometer beneath the interface.



**Figure 3:** Quantum effects in advanced MOS transistors. (Advanced MOS transistors fabricated with current technologies are yet influenced by quantum effects since they are already operating in the sub 100nm range. Quantum effects are mostly parasitics and influence the classical expected device behaviour negatively due to treshold voltage shift, gate capacitance degradation and gate dielectric tunneling current. Since mos devices are ubiquitously used in digital and analog circuits, the circuit aspect of quantum effects has to be modeled properly by means of quantum corrected compact models.)

# **Quantum Transport**

The natural extension of the semi-classical transport models to quantum physics consits of the Wigner equation, or equivalently of a system of infinitely many Schrödinger equations.

The single-particle effective mass Schrödinger equation can describe only a situation in which the electrons move perfectly coherently throughout the device. Any loss of coherence due to inelastic collisions requires a higher-level description. In the viewpoint of scattering, we need a method to determine the transmission and reflection coefficients for any given energy. These are determined by solving, either explicitly or implicitly the Schrödinger equation. The *transmission matrix approach* [4] solves the Schrödinger equation implicitly. In practical calculations, the transmission matrix approach have proved to be less then satisfactory, because it is prone to arithmetic overlfow. A much more robust and effective scheme for solving the Schrödinger equation is the *quantum transmitting boundary method* [5, 6] which solves the Schrödinger equation explicitly.

# References

- [1] S. Teitel and J. Wilkins, "Ballistic transport and velocity overshoot in semiconductors: Part i uniform field effects," *Electron Devices, IEEE Transactions on*, vol. 30, no. 2, pp. 150–153, Feb 1983.
- [2] A. Svizhenko, M. Anantram, and T. Govindan, "Ballistic transport and electrostatics in metallic carbon nanotubes," *Nanotechnology, IEEE Transactions on*, vol. 4, no. 5, pp. 557–562, Sept. 2005.
- [3] C. Falco, E. Gatti, A. Lacaita, and R. Sacco, "Quantum-corrected drift-diffusion models for transport in semiconductor devices," *Journal of Computational Physics*, vol. 204, pp. 533–561, 2005.
- [4] Y. Ando and T. Itoh, "Calculation of transmission tunneling current across arbitrary potential barriers," *Journal of Applied Physics*, vol. 61 (4), pp. 1497–1502, 1987.
- [5] C. S. Lent and D. J. Kirkner, "The quantum transmitting boundary method," *Journal of Applied Physics*, vol. 67 (10), pp. 6353–6359, 1990.
- [6] M. Baro, N. B. Abdallah, P. Degond, and A. El Ayyadi, "A 1d coupled schrodinger drift-diffusion model including collisions," *Journal of Computational Physics*, vol. 203, no. 1, pp. 129–153, Feb. 2005.

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