Current Transport Models for Nano-Scale Semiconductor Devices

Andreas Gehring and Siegfried Selberherr
Institute for Microelectronics, TU Vienna
Gusshausstr. 27–29, A-1040 Vienna, Austria
E-mail: Selberherr@TUWien.ac.at

ABSTRACT

An overview of models for the simulation of current transport in micro- and nanoelectronic devices within the framework of TCAD applications is presented. Starting from macroscopic transport models, currently discussed enhancements are specifically addressed. This comprises the inclusion of higher-order moments into the transport models, the incorporation of quantum correction and tunneling models up to dedicated quantum-mechanical simulators, and mixed approaches which are able to account for both, quantum interference and scattering. Specific TCAD requirements are discussed from an engineer's perspective and an outlook on future research directions is given.

Keywords: Device Simulation, TCAD, Transport Models

1. INTRODUCTION

The continuous minimum feature size reduction of microelectronic devices, institutionalized by the ITRS roadmap [1], has been partly enabled by the support of sophisticated Technology CAD (TCAD) tools. These tools promise to assist process and device engineers during all stages of development, ranging from process simulation to device and circuit simulation. Today, device engineers face the challenge to move from the *microelectronic* feature scale in the mid-90's, with typical MOSFET gate lengths just entering the sub-micron region, to the realm of *nanoelectronics* with 90 nm gate length devices in volume production and 6 nm gate length transistors fabricated in research labs [2]. The continuum approximation, already questioned in the mid-1990's, has to be abandoned in this regime, and different approaches for the simulation of devices in the nanometer regime have been proposed.

In general, the inaccuracies of presently applied semiclassical macroscopic transport models are due to non-local effects [3], either caused by classical or quantum-mechanical non-localities. Classical non-localities arise because the distribution of electrons in very small devices does not depend on local quantities alone. Quantum-mechanical non-localities occur due to the wave nature of electrons and the occurrence of quantization, either due to high electric fields as in the inversion layer of a MOSFET, or due to the geometry as in ultrasmall double-gate or FinFET devices.

Fig. 1 depicts the hierarchy of models which are currently used for the description of current transport. Semiclassical transport models rely on classical states characterized by a distribution function which is governed by the Boltzmann transport equation. In Section 2 we will give a review of the evolution of current semiclassical transport models, and present recent results achieved with higher-order transport models. Quantum ballistic transport is based on pure states described by a wave function, the evolution of which follows Schrödinger's equation. These approaches are mainly used for the simulation of closed systems, such as quantum corrections in the inversion layer of MOSFETs. In Section 3, these quantum-ballistic transport approaches will be described. Finally, quantum transport theory deals with mixed states. There exist different formulations, which can be based on the Dyson equation, the Liouville/von Neumann equation, or the Wigner transport equation. Section 4 deals with these approaches, which are characterized by both scattering and quantization. A conclusion will summarize the main findings and give directions for future research.

2. SEMICLASSICAL TRANSPORT

In the early days of semiconductor technology, the electrical characteristics of semiconductor devices could be estimated based on simple analytic compact models, employing a variety of simplifying approximations but capturing the basic physical principles of carrier transport. These models were based on the drift-diffusion (DD) formalism, where the current in the device is governed by the electric field and the concentration gradients alone. Based on the ground-breaking work of Scharfetter and Gummel [4], who first proposed a robust discretization scheme for the drift-diffusion equations, the numerical simulation of semiconductor devices was enabled. Computer programs such as Minimos [5] and Pisces [6] have been developed and played a pioneering role in the deeper understanding of current transport for engineering purposes and in the development of miniaturized devices. For the first time, it was possible to provide insight into the functioning of semiconductor devices by means of the distribution of internal device quantities, instead of global quantities such as current-voltage characteristics. Since then, numerous transport models of increasing complexity have been proposed. All models are coupled to the Poisson equation

$$\nabla \cdot (\kappa \nabla \phi) = \rho(\phi) \,, \qquad \rho(\phi) = \mathrm{q}(n - p - C) \qquad (1)$$

where ϕ denotes the electrostatic potential and κ the dielectric permittivity. The question of current transport ba-

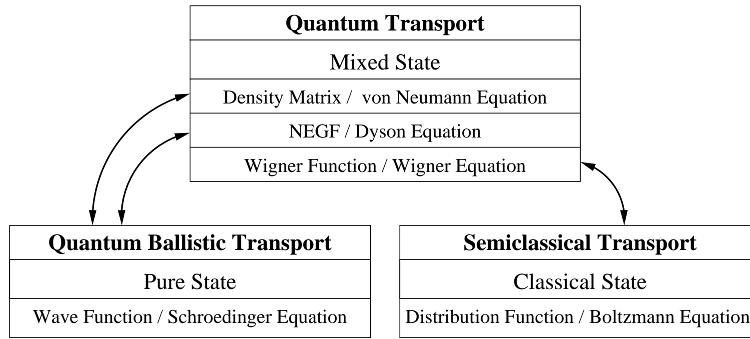

Figure 1: Hierarchy of transport equations in semiconductor current transport modeling.

sically reduces to the self-consistent modeling of the nonlinear charge density $\rho(\phi)$ in (1), which includes the electron and hole concentration, the net concentration of impurities, and other charges such as ionized traps.

Neglecting the quantum-mechanical nature of electrons, carrier transport in a device is described by Boltzmann's transport equation, a seven-dimensional integro-differential equation in phase space [7]

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_r f + \frac{s_\nu \, \mathrm{q} \, \mathbf{E}}{\hbar} \cdot \nabla_{\mathbf{k}} f = \left(\frac{\partial f}{\partial t} \right)_{\mathrm{coll}} . \quad (2)$$

Here, $f(\mathbf{r}, \mathbf{k}, t)$ is the distribution of carriers in space ($\mathbf{r}$), momentum ($\hbar\mathbf{k}$), and time. The charge sign s_ν ($\nu = n, p$) distinguishes between electrons and holes. On the right-hand side stands the collision operator which describes scattering of particles due to phonons, impurities, interfaces, or other scattering sources. However, for realistic structures, the direct solution of this equation is computationally prohibitive. It is rather solved by approximate means applying the method of moments or using Monte Carlo methods.

2.1. The Method of Moments

In the method of moments each term of (2) is multiplied with a weight function and integrated over $\mathbf{k}$-space. This yields a set of differential equations in the $(\mathbf{r}, t)$-space. The moments of the distribution function are defined as

$$\langle \Phi \rangle = \frac{1}{4\pi^3} \int \Phi \, f(\mathbf{r}, \mathbf{k}, t) \, \mathrm{d}^3 k \, . \quad (3)$$

This generates an infinite set of equations which must be closed by a suitably chosen ansatz [8]. Closure after the second moment and assuming a cold Maxwellian distribution leads to the drift-diffusion equations, which for electrons read

$$\nabla \cdot \mathbf{J}_n = \mathrm{q}R + \mathrm{q}\frac{\partial n}{\partial t} \, , \quad (4)$$

$$\mathbf{J}_n = \mathrm{q}n\mu_n \mathbf{E} + \mathrm{q}D_n \nabla n \, . \quad (5)$$

In these equations $\mathbf{J}_n$ denotes the current density, R the net recombination rate, μ_n the mobility, $\mathbf{E}$ the electric field, and D_n the diffusion coefficient. Together with (1), a coupled equation system is formed which is solved numerically by means of the box integration method.

From an engineering point of view, the drift-diffusion model has proven amazingly successful due to its efficiency, numerical robustness, and the feasibility to perform two- and three-dimensional studies on fairly large unstructured grids. However, several shortcomings of this model are critical for miniaturized devices. Especially hot-carrier effects such as impact ionization or velocity overshoot motivated the development of higher-order transport models such as the hydrodynamic, energy-transport, and six-moments model [9]. These models allow the electron energy distribution function to be described beyond the Maxwellian approximation, and they are used routinely in commercial and academic device simulators.

2.2. The Monte Carlo Method

The Monte Carlo method is well established for studying semiconductor devices and exploring semiconductor properties. The method simulates the motion of charge carriers in the six-dimensional phase space formed by position and momentum. Subjected to the action of an external force field, the point-like carriers follow trajectories governed by Newton's law and the carrier's dispersion relation. These drift processes are interrupted by scattering events which are assumed local in space and instantaneous in time. The duration of a drift process, the type of scattering mechanism, and the state after scattering are selected randomly from given probability distributions which are characteristic to the microscopic scattering process. As a calibration tool, the full-band Monte Carlo method has gained widespread acceptance, since it precisely accounts for the band structure of the considered semiconductor [10]. Fig. 2 shows a comparison of different macroscopic simulation approaches with full-band Monte Carlo results for a 250 nm and a 50 nm double-gate MOSFET [11]. It can be seen that transport models based on two, four, and six moments deliver similar results for the long-channel device, while only the six moments model is able to reproduce the full-band Monte Carlo results for the short-channel device. Applying the energy-transport model in this case yields almost no improvement over the drift-diffusion model.

The Monte Carlo method has been enhanced to account for quantum effects using an effective potential instead of the self-consistent potential determined by the Poisson equa-

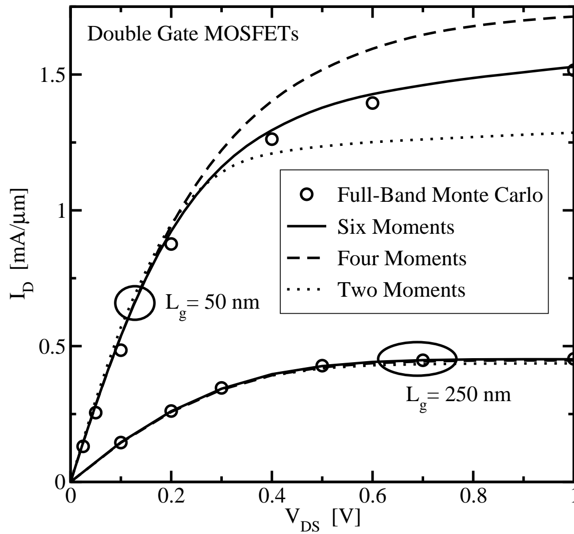

Figure 2: Comparison of macroscopic transport models with full-band Monte Carlo. While all models yield similar results at large gate lengths, only the six-moments model reproduces the short-channel Monte Carlo results.

tion [12], [13]. The effective potential can be obtained by a convolution of the electrostatic potential with a Gaussian function which leads to a smoothing of the original potential. A quantum correction based on the Schrödinger equation applied to a full-band Monte Carlo simulator is reported in [14].

3. QUANTUM-BALLISTIC TRANSPORT

Within macroscopic transport models presented above, quantum-mechanical effects are usually accounted for by means of quantum corrections. The fabrication of structures in the nanometer regime makes this approach questionable and motivated the development of quantum-mechanical modeling tools which calculate the carrier concentration by purely quantum-mechanical principles. They became especially important for the evaluation of gate dielectrics, which represent the smallest feature scale in microelectronics. Neglecting quantum confinement in this regime leads to results which are not just slightly inaccurate, but systematically wrong. As an example, the CV-characteristics of an 1.5 nm dielectric layer is shown in Fig. 3 for different poly doping concentrations calculated classically and quantum-mechanically, showing a large discrepancy. One-dimensional closed-boundary quantum simulators are today established tools for the characterization of gate dielectric layers [15]–[17]. Such one-dimensional solutions of the Schrödinger equation are also frequently used to derive correction factors for the carrier concentration calculated by macroscopic transport models [18]–[20]. They can be used to yield a quick estimate of quantum-confinement related effects without degrading the efficiency of the device simulator used. However, since they are based on the closed-boundary Schrödinger equation charge transport is neglected. Thus, they are not applicable to open systems characterized by thin or low energy barriers, which give rise to complex eigenvalues and, as a consequence, charge transport by tunneling.

3.1. Tunneling Models

Quantum-ballistic tunneling models are still predominantly applied for the simulation of gate leakage in CMOS devices. Here, the central quantity is the quantum-mechanical transmission coefficient $TC(\mathcal{E})$ which is used in the so-called Tsu-Esaki equation

$$J = \frac{4\pi m_{\mathrm{eff}}\mathrm{q}}{h^3} \int_{\mathcal{E}_{\min}}^{\mathcal{E}_{\max}} TC(\mathcal{E}_x) N(\mathcal{E}_x)\,\mathrm{d}\mathcal{E}_x \tag{6}$$

to calculate the tunneling current density. Methods such as the Wentzel-Kramers-Brillouin (WKB), the transfer-matrix, or quantum transmitting boundary method have been proposed to calculate the transmission coefficient [21]. The resulting tunneling currents can be easily incorporated into macroscopic transport models by means of additional generation/recombination processes in (4).

However, the further reduction of channel lengths raises the question for a fully quantum-mechanical treatment of carrier transport. This makes the solution of Schrödinger's equation with open boundary conditions necessary, which can be done by means of the quantum transmitting boundary method as shown in [22], [23]. An established and sophisticated framework for these calculations is the non-equilibrium Green's Function method, which is predominantly used for one-dimensional studies of resonant tunneling diodes [24]. If a system is characterized by a specific confinement direction, two- and three-dimensional quantum ballistic simulations can efficiently be performed by means of an adiabatic decomposition [25], [26].

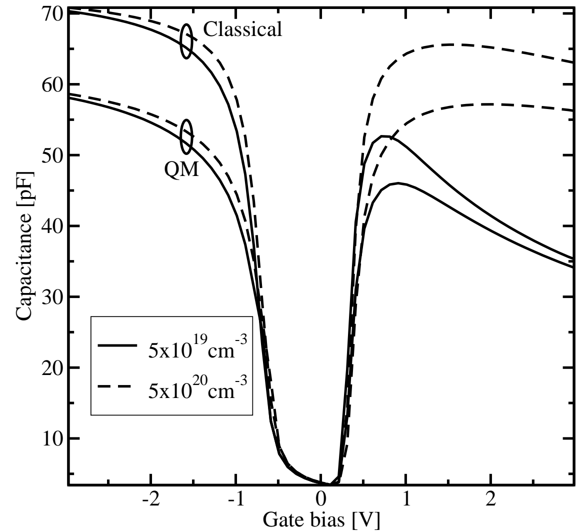

Figure 3: Comparison of CV characteristics of a 1.5 nm dielectric layer with different polysilicon doping applying classical and quantum-mechanical simulations.