



Evolution of Current Transport Models for Engineering Applications

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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 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.

Figure 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 semiclassical transport models, and describe recent results with regard to 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 quantum transport characterized by both scattering and quantization. A conclusion will

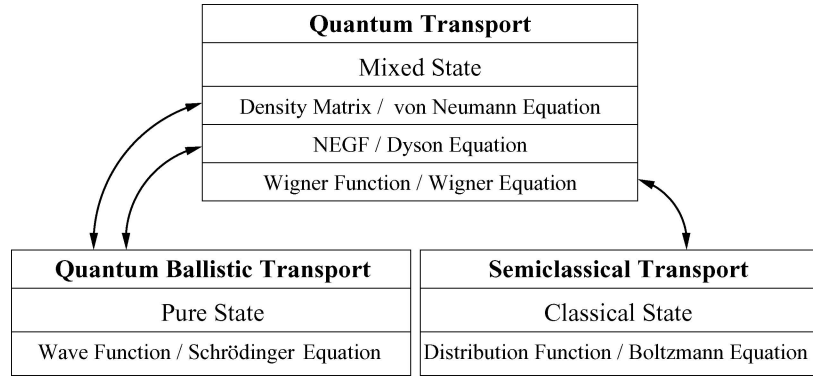


Figure 1. Hierarchy of transport equations in semiconductor current transport modeling.

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

$$\nabla \cdot (\kappa \nabla \phi) = \rho(\phi), \quad \rho(\phi) = q(n - p - C) \quad (1)$$

where ϕ denotes the electrostatic potential and κ the dielectric permittivity. The question of current transport basically reduces to the self-consistent modeling of the non-linear 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]

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{r}} f - \frac{q\mathbf{E}}{\hbar} \cdot \nabla_{\mathbf{k}} f = \left(\frac{\partial f}{\partial t} \right)_{\text{coll}}. \quad (2)$$

Here, $f(\mathbf{r}, \mathbf{k}, t)$ is the distribution of carriers in space (\mathbf{r}), momentum ($\hbar\mathbf{k}$), and time. 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. 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

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

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

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

$$\mathbf{J}_n = qn\mu_n \mathbf{E} + qD_n \nabla n. \quad (5)$$

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, this 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 [8]. 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. As a calibration tool, the full-band Monte Carlo method has become accepted, since it can precisely account for the various scattering processes in the scattering operator [9]. Figure 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 [10]. It can be seen that transport models based on two, four, and six moments deliver sim-

ilar 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.

3. Quantum-Ballistic Transport

Within the macroscopic transport models presented above, quantum-mechanical effects are usually accounted for by means of quantum corrections in the continuity equations. However, the fabrication of structures in the nanometer regime triggered the development of quantum-mechanical modeling tools. This 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 and showing a large discrepancy under inversion conditions. This apparent inaccuracy of conventional models justified the development of one-dimensional quantum device simulators which are today established tools for the characterization of gate dielectric layers [11–13]. Such one-dimensional solutions of the Schrödinger equation are also frequently used to derive correction factors for the carrier concentration

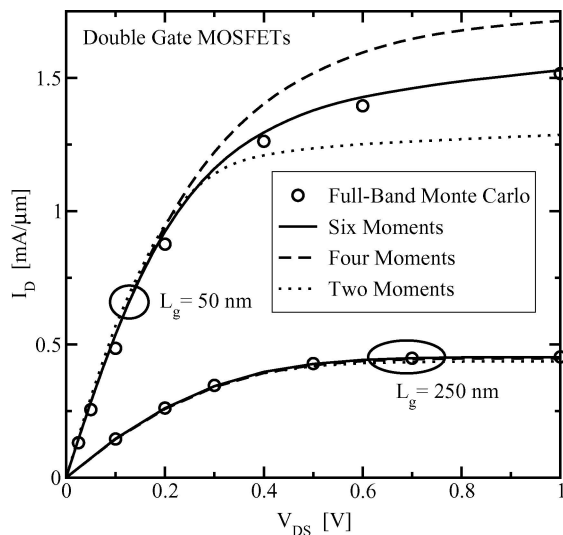


Figure 2. Comparison of macroscopic transport models with full-band Monte Carlo [10]. While all models yield similar results at large gate lengths, only the six-moments model reproduces the short-channel Monte Carlo results.

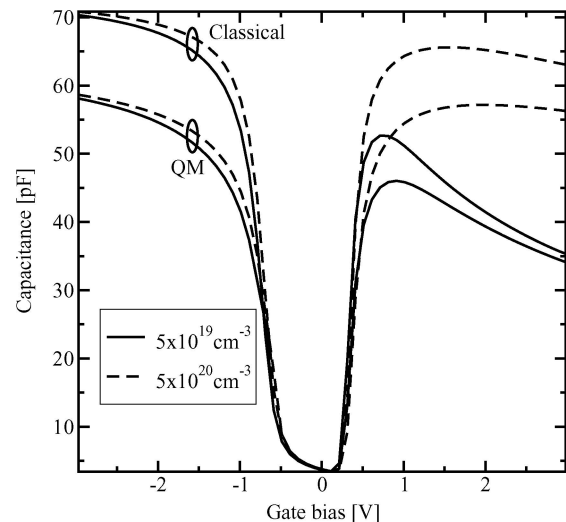


Figure 3. Comparison of CV characteristics of a 1.5 nm dielectric layer with different polysilicon doping applying one-dimensional classical and quantum-mechanical simulations.

calculated by macroscopic transport models [14–16]. They can be used to yield a quick estimate of quantum-confinement related effects without degrading the efficiency of the device simulator used. However, based on the closed-boundary Schrödinger equation charge transport is neglected.

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

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

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 [17]. 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 [18,19]. 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 [20]. Two- and three-dimensional quantum ballistic simulations can be performed by means of an adiabatic decomposition of wave functions into one or two confinement directions [21,22]. Recently, simulators accounting for a full two-dimensional solution of the open-boundary Schrödinger equation have been reported and applied to the simulation of 10 nm double-gate MOSFETs [23,24]. Besides the requirement for a fine and sometimes even equidistant mesh, a main obstacle in these approaches is that the treatment of scattering is not straightforwardly possible. Furthermore, these simulators are usually limited to specific geometries, restrictive grids, or small length scales, which makes their usability for engineering applications questionable. Nevertheless, these simulation approaches are necessary for the estimation

of upper bounds of current transport at the quantum limit.

4. Quantum Transport

The methods described so far are either based on the assumption of pure classical or pure quantum transport. Modern microelectronic devices, however, are characterized by the transition between large reservoirs with strong carrier scattering, and small regions where quantum effects are important or even dominate. To first order, quantum correction models can account for these effects. A more rigorous approach is to consider models derived from the Wigner equation. The Wigner function is given by a transformation of the density matrix [25,26]

$$f_w(\mathbf{r}, \mathbf{k}, t) = \int \rho\left(\mathbf{r} + \frac{\mathbf{s}}{2}, \mathbf{r} - \frac{\mathbf{s}}{2}, t\right) \exp(-i\mathbf{k} \cdot \mathbf{s}) ds.$$

The kinetic equation for the Wigner function is the Wigner transport equation which is similar to the Boltzmann equation except the Wigner potential at the right-hand side

$$\begin{aligned} & \left(\frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla_r + \frac{q\mathbf{E}}{\hbar} \cdot \nabla_k \right) f_w \\ & = \int V_w(\mathbf{r}, \mathbf{k} - \mathbf{k}') f_w(\mathbf{k}', \mathbf{r}, t) d\mathbf{k}' + \left(\frac{\partial f_w}{\partial t} \right)_{\text{coll}}. \end{aligned} \quad (7)$$

The Wigner potential is defined by

$$\begin{aligned} V_w(\mathbf{r}, \mathbf{k}) = & \frac{1}{i\hbar (2\pi)^3} \int \left(V\left(\mathbf{r} + \frac{\mathbf{s}}{2}\right) \right. \\ & \left. - V\left(\mathbf{r} - \frac{\mathbf{s}}{2}\right) \right) \exp(-i\mathbf{k} \cdot \mathbf{s}) ds. \end{aligned} \quad (8)$$

From this equation the quantum drift-diffusion or quantum hydrodynamic models can be derived applying the method of moments [27]. It is therefore more suitable for the implementation in device simulators than a Schrödinger-POISSON solver which strongly depends on non-local quantities. However, it was reported that, while the carrier concentration in the inversion layer of a MOSFET can be modeled correctly, the method fails to reproduce tunneling currents [28].

Therefore, strong efforts have been undertaken to couple the most accurate classical device simulation approach, the Monte Carlo technique, with quantum-mechanical formulations [29–31]. One possibility is

to use an effective potential instead of the solution of POISSON's equation in the Monte Carlo simulation [32,33]. That can be achieved by a convolution of the electrostatic potential with a GAUSSIAN function which leads to a smoothing of the original potential.

A less heuristic approach is to solve the WIGNER transport Eq. (7) by means of Monte Carlo techniques. Unlike classical distribution functions, however, the WIGNER function permits positive and negative values. Therefore, it cannot be interpreted as a probability distribution function, a peculiarity known as the *negative sign problem*. Instead, the Wigner function can be modeled as the difference of two positive functions which describe in-scattering and out-scattering of particles. This approach has the advantage that it allows for a seamless transition between classical and quantum-mechanical regions in a device [31]. This method has been applied to the simulation of resonant tunneling diodes as shown in Fig. 4 and it was recently used for the simulation of 10 nm double-gate MOSFETs [34].

A typical application of quantum transport interesting for device engineers is shown in Fig. 5, depicting a cross-section through the channel of different multi-gate silicon-on-insulator devices, namely a FinFET (top) and a Π -gate FET (bottom) [35]. Three-dimensional device simulations have been performed for turned-off devices ($V_{DS} = 1.0$ V, $V_{GS} = 0.0$ V) by means of coupling a two-dimensional Schrödinger-Poisson solver to the device simulator

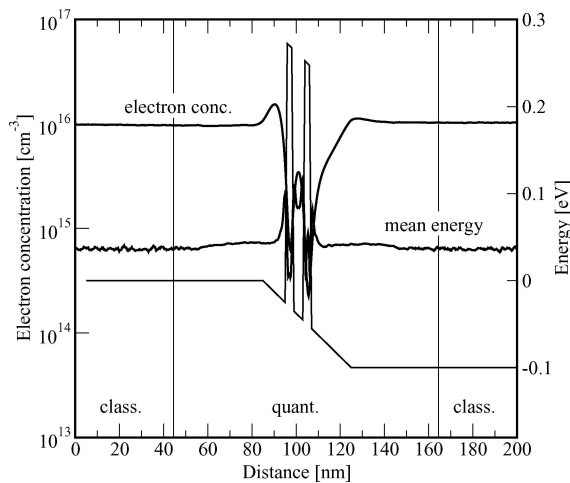


Figure 4. Wigner Monte Carlo results of electron concentration and mean energy for a resonant tunneling diode [31].

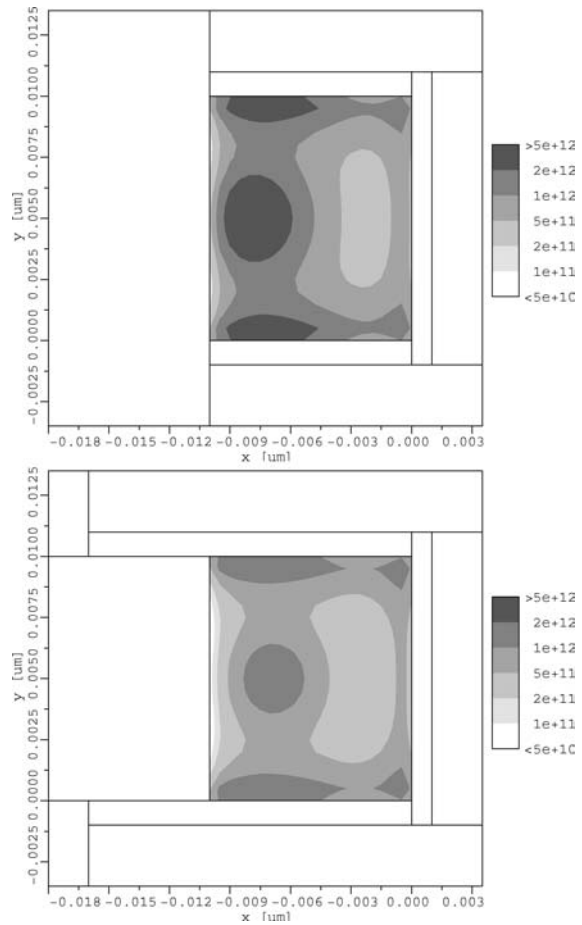


Figure 5. Carrier concentration in the middle of the channel of a turned-off triple-gate FinFET (top) and a Π -FET [35] (bottom). The Π -gate efficiently suppresses the spurious drain field.

MINIMOS-NT [36], and the figures show the resulting carrier concentrations. While only the gate-all-around structure can fully deplete the channel, the Π -gate FET efficiently shields the channel from the drain bias, while posing only moderate additional process complexity.

5. Conclusions

Semiconductor physics is a vast field and simulation approaches abound. Physicists are often tempted to use overly complicated approaches, in an understandable effort not to lose the important physics. However, some constraints for engineering application should be kept in mind. Models must be efficient: Timely results are more valuable than accurate analyses [37]. There is a

need for three-dimensional simulations, even if they are only rarely applied to check for spurious effects. Device simulators must allow a coupling with process simulators, since a detailed, physics-based transport model is of no use if geometry and doping are not described correctly. Therefore, support of unstructured grids is necessary. Furthermore, the simulators should be general-purpose and not limited to specific geometries or simulation modes. It is still not clear which of the outlined quantum transport approaches will find its way into integrated TCAD environments, but its further success depends on efficient and accurate modeling of these new effects.

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References

1. "International Technology Roadmap for Semiconductors - 2003 Edition," (2003), <http://public.itrs.net>.
2. H. Iwai, "CMOS downsizing toward Sub-10 nm," *Solid-State Electron*, **48**(4), 497 (2004).
3. F.O. Heinz et al., "Quantum transport phenomena and their modeling," in *Symposium on Nano Device Technology* (2004) p. 2.
4. D.L. Scharfetter and H.K. Gummel, "Large-signal analysis of a silicon read diode oscillator," *IEEE Trans. Electron Devices*, **16**(1), 64 (1969).
5. S. Selberherr et al., "MINIMOS—A program package to facilitate MOS device design and analysis," in *Numerical Analysis of Semiconductor Devices and Integrated Circuits* (1979) p. 275.
6. M.R. Pinto, *PISCES IIB*, Stanford University (1985).
7. S. Selberherr, *Analysis and Simulation of Semiconductor Devices*, Springer (1984).
8. T. Grasser et al., "A review of hydrodynamic and energy-transport models for semiconductor device simulation," *Proc. IEEE*, **91**(2), 251 (2003).
9. M.V. Fischetti and S.E. Laux, "Monte carlo analysis of electron transport in small semiconductor devices including band-structure and space-charge effects," *Physical Review B*, **38**(14), 9721 (1988).
10. T. Grasser et al., "Advanced transport models for sub-micrometer devices," in *Proc. Intl. Conf. on Simulation of Semiconductor Processes and Devices* (2004), p. 8.
11. S. Jallepalli et al., "Electron and hole quantization and their impact on deep submicron silicon p- and n-MOSFET characteristics," *IEEE Trans. Electron Devices*, **44**(2), 297 (1997).
12. D. Vasileska et al., "Scaled silicon MOSFET's: Degradation of the total gate capacitance," *IEEE Trans. Electron Devices*, **44**(4), 584 (1997).
13. E.M. Vogel et al., "A capacitance-voltage model for polysilicon-gated MOS devices including substrate quantization effects based on modification of the total semiconductor charge," *Solid-State Electron*, **47**, 1589 (2003).
14. W. Hänsch et al., "Carrier transport near the Si/SiO₂ interface of a MOSFET," *Solid-State Electron*, **32**(10), 839 (1989).
15. M.J. van Dort et al., "A simple model for quantization effects in heavily-doped silicon MOSFETs at inversion conditions," *Solid-State Electron*, **37**(3), 411 (1994).
16. C. Jungemann et al., "Improved modified local density approximation for modeling of size quantization in NMOSFETs," in *Proc. Intl. Conf. Modeling and Simulation of Microsystems* (2001).
17. A. Gehring, *Simulation of Tunneling in Semiconductor Devices*, Dissertation, Technische Universität Wien (2003).
18. C.S. Lent and D.J. Kirkner, "The quantum transmitting boundary method," *J. Appl. Phys.*, **67**(10), 6353 (1990).
19. W.R. Frensley, "Numerical evaluation of resonant states," *Superlattices & Microstructures*, **11**(3), 347 (1992).
20. R. Lake et al., "Single and multiband modeling of quantum electron transport through layered semiconductor devices," *J. Appl. Phys.*, **81**(12), 7845 (1997).
21. F.O. Heinz et al., "Full quantum simulation of silicon-on-insulator single-electron devices," *J. Computational Electronics*, **1**(1), 161 (2002).
22. G. Curatola et al., "Modeling and simulation challenges for nanoscale MOSFETs in the ballistic limit," *Solid-State Electron*, **48**(4), 581 (2004).
23. S.E. Laux et al., "Ballistic FET modeling using QDAME: Quantum device analysis by modal evaluation," *IEEE Trans. Nanotechnology*, **1**(4), 255 (2002).
24. M. Sabathil et al., "Towards fully quantum mechanical 3D device simulations," *J. Computational Electronics*, **1**, 81 (2002).
25. E. Wigner, "On the quantum correction for thermodynamic equilibrium," *Physical Review*, **40**, 749 (1932).
26. H. Kosina and M. Nedjalkov, "Wigner function based device modeling," in *Handbook of Theoretical and Computational Nanotechnology*, Springer (2005).
27. A. Wettstein et al., "Quantum device-simulation with the density-gradient model on unstructured grids," *IEEE Trans. Electron Devices*, **48**(2), 279 (2001).
28. T. Hoehr et al., "On density-gradient modeling of tunneling through insulators," in *Proc. Intl. Conf. on Simulation of Semiconductor Processes and Devices* (2002) pp. 275–278.
29. L. Shifren et al., "A wigner function-based quantum ensemble monte carlo study of a resonant tunneling diode," *IEEE Trans. Electron Devices*, **50**(3), 769 (2003).
30. B. Winstead and U. Ravaioli, "A quantum correction based on schrödinger equation applied to monte carlo device simulation," *IEEE Trans. Electron Devices*, **50**(2), 440 (2003).
31. H. Kosina et al., "A Monte Carlo method seamlessly linking quantum and classical transport calculations," *J. Computational Electronics*, **2**(2–4), 147 (2002).
32. Y. Li et al., "Modeling of quantum effects for ultrathin Oxide MOS structures with an effective potential," *IEEE Trans. Nanotechnology*, **1**(4), 238 (2002).

33. K.Z. Ahmed et al., "On the evaluation of performance parameters of MOSFETs with alternative gate dielectrics," *IEEE Trans. Electron Devices*, **50**(12), 2564 (2003).
34. A. Gehring and H. Kosina, "Wigner-function based simulation of classic and ballistic transport in scaled DG-mosfets using the Monte Carlo method," in (2004).
35. J.-T. Park et al., "Pi-Gate SOI MOSFET," *IEEE Electron Device Lett*, **22**(8), 405 (2001).
36. Institut für Mikroelektronik Technische Universität Wien, Austria, *MINIMOS-NT 2.1 User's Guide* (2004).
37. M. Duane, "TCAD needs and applications from a users perspective," *IEICE Trans. Electron*, **E82-C**(6), 976 (1999).