Modeling Current Transport in Ultra-Scaled Field Effect Transistors

Viktor Sverdlov, Hans Kosina, and Siegfried Selberherr

Abstract— An overview of models for the simulation of current transport in micro- and nanoelectronic devices within the framework of TCAD applications is presented. Modern enhancements of macroscopic transport models based on microscopic theories 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.

I. Introduction

The impressive increase in computational performance and speed of integrated circuits in the past decades has been mostly enabled by the aggressive size reduction of microelectronic devices. This trend is expected to continue in the coming decade as it is institutionalized by the International Technology Roadmap for Semiconductors [1]. Today, when the 90 nm technology node with physical transistor gate lengths in the range of 40 nm is in mass production and the 6 nm gate length transistor has been demonstrated in research labs [2], [3], the device engineers are facing the challenge to introduce the 65 nm technology node already in a year. New technology nodes are introduced every 3 years, with a long-term projection of the 22 nm node to be in production by the year 2016.

Technology CAD (TCAD) tools are designed to assist in development and engineering at all stages ranging from process simulation to device and circuit analysis. Due to the aggressive downscaling of device feature sizes, inaccuracies of presently applied TCAD tools based on semiclassical macroscopic transport models appear. The origin of these inaccuracies stems from the non-local nature of carrier propagation in ultra-scaled devices [4]. The non-local effects may be of classical or quantum-mechanical nature, depending on the underlying microscopic physics relevant to the transport process. Classical non-localities appear when the mean-free path is getting comparable to the device feature size. In this case hot carrier effects are becoming important. Quantum mechanical non-local effects start to determine the transport properties when the device size is of the order of the De-Broglie electron wave length. Size quantization of carrier motion in surface inversion layers of MOSFETs and in ultra-scaled multi-gate devices as well as the tunneling current including gate leakage are the most important examples of quantum effects in MOSFETs.

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Fig. 1 shows the hierarchy and mutual interrelation of current transport models presently used for device modeling. Semiclassical transport models are based on the Boltzmann equation which includes scattering integrals describing realistic microscopic processes. These purely classical models, augmented with quantum corrections, are still of great importance due to their relative simplicity, computational robustness, and an ability to provide reasonable quantitative results within seconds even for devices with gate length as short as 50 nm. They may serve well for engineering and optimization of 90 nm node devices. A brief overview of the currently developed semiclassical transport models will be presented in Section 2.

Quantum ballistic transport models describe a coherent propagation of carriers. They are based on the solution of the Schrödinger equation for the wave function, supplemented with the corresponding boundary conditions. This approach is efficient and provides accurate results when carrier scattering is irrelevant and can be neglected. The method will be illustrated in Section 3 by an example of transport in carbon nanotubes where transport is coherent [5].

Finally, quantum transport theory represents the full quantum-mechanical description, which combines the coherent carrier motion between scattering with the coherence (or phase) breaking due to carrier scattering. Different formalisms are currently used, based on the Dyson equation for the non-equilibrium Green's functions, the quantum Liouville/von Neumann equation, or the Wigner transport equation. Section 4 deals with quantum transport characterized by both scattering and quantization. A conclusion will summarize the main findings and give directions for future research.

II. Semiclassical Transport

After the ground-breaking work of Scharfetter and Gummel [6], who first proposed a robust discretization scheme for the drift-diffusion equation, computer programs like

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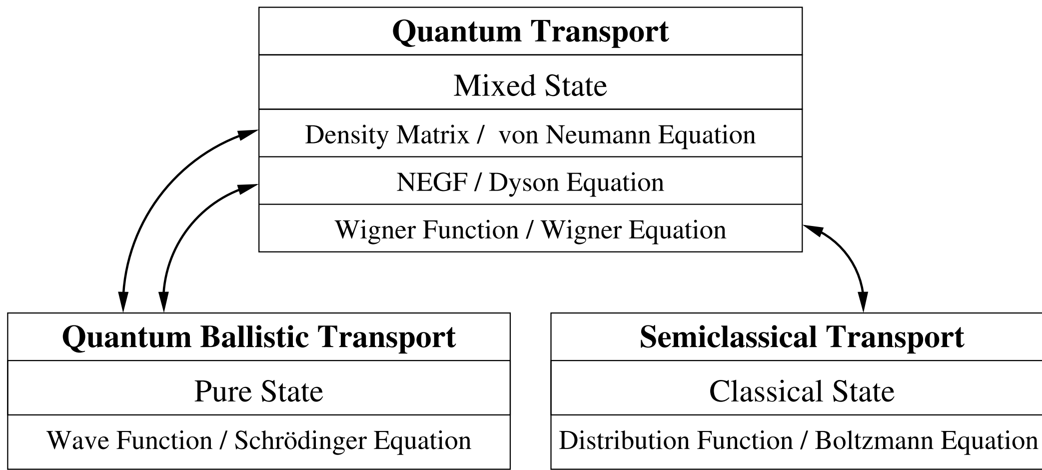

Fig. 1. Hierarchy of transport equations in semiconductor current transport modeling.

Minimos [7] and Pisces [8] played a pioneering role in numerical simulations of current transport properties of semiconductor device engineering. Since then, numerous transport models of increasing complexity have been introduced. The semiclassical transport description is based on the Boltzmann equation for the distribution of carriers $f(\mathbf{r},\mathbf{k},t)$ in the point $(\mathbf{r},\mathbf{k})$ of phase space

$$\frac{\partial f}{\partial t} + \mathbf{v}\cdot\nabla_r f - \frac{\mathrm{q}\mathbf{E}}{\hbar}\cdot\nabla_{\mathbf{k}} f = \left(\frac{\partial f}{\partial t}\right)_{\mathrm{coll}}, \quad (1)$$

where the collision integral on the right-hand side describes carrier scattering due to phonons, impurities, interfaces, or other scattering sources. Although the solution of the Boltzmann equation can be found numerically by means of Monte Carlo (MC) methods, TCAD models based on moments of the distribution function $f(\mathbf{r},\mathbf{p},t)$ are highly desirable. Being computationally significantly less expensive than the MC method, these higher-order moments methods provide a reasonable quantitative answer for devices as short as 50 nm within seconds. The reason for good results stems from the fact that the higher-order moments models already take into account a deviation of $f(\mathbf{r},\mathbf{k},t)$ from the Maxwellian distribution. Multiplying (1) with $\mathbf{k^n}$ on both sides and integrating it over $\mathbf{k}$, an infinite set of differential equations relating moments of different order n

$$\langle\mathbf{k}^n\rangle = \frac{1}{4\pi^3}\int \mathbf{k}^n\, f(\mathbf{r},\mathbf{k},t)\,\mathrm{d}^3k \quad (2)$$

is obtained. By assuming the cold Maxwellian distribution, the second moment is only expressed via the moments of a lower order and one obtains a closed set of equations relating the density to the current, which is the famous drift-diffusion model. The fairly new six moments model [9] naturally takes into account hot-carrier effects such as avalanche generation, hot carrier induced gate currents, or hot-carrier diffusion, which typically take place in a Silicon-On-Insulator (SOI) floating body MOSFET. The full-band MC method is often accepted as a calibration tool , since it can precisely account for the various scattering processes in the scattering operator [10]. Fig. 2 shows a comparison of different macroscopic simulation approaches with the microscopic full-band MC results for a 250 nm and a 50 nm double-gate MOSFET [11]. While the transport models based on two, four, and six moments give similar results for the long-channel classical device, only the six moments model is able to capture the classical non-local effects in 50 nm gate length devices and to reproduce the full-band MC result.

Another important development of transport models is related to the MC method for solving the Boltzmann equation. Kurosawa in 1966 [12] is considered to be the first who applied the MC method to simulate the transport in semiconductor. Later the significantly improved MC method was successfully applied to transport description in a variety of semiconductors [13]. For electrons in silicon, the most thoroughly investigated case, it is believed that a satisfactory understanding of the band structure and of the basic scattering mechanisms has been achieved giving rise to a “standard model” [14]. Nowadays, an accurate MC evaluation of carrier transport properties in surface inversion layers is of primary importance for improving performance of modern CMOS bulk devices. Due to the strong confinement of carriers in the inversion layer of bulk MOSFETs or due to the geometric confinement in modern multi-gate FETs the carrier motion is getting quantized in the confinement direction giving rise to the formation of quantum subbands. One possibility to address the quantum effects due to confinement is to use an effective potential instead of the solution of the Poisson equation in the three-dimensional MC simulation. This can also be achieved by a convolution of the electrostatic potential with a Gaussian function, which leads to a smoothing of the original potential [15], [16], [17]. Another option is to use the self-consistent Poisson-Schrödinger-based quantum corrected potential [18], [19]. These approaches combine advantages

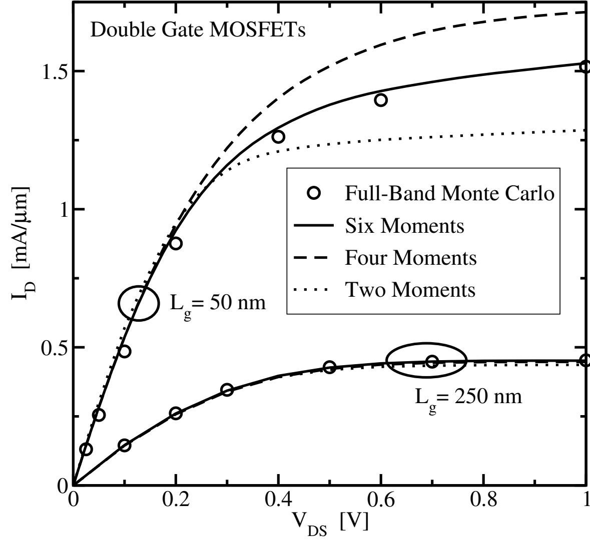

Fig. 2. Comparison of macroscopic transport models with full-band Monte Carlo [11]. While all models yield similar results at large gate lengths, only the six-moments model reproduces the short-channel Monte Carlo results.

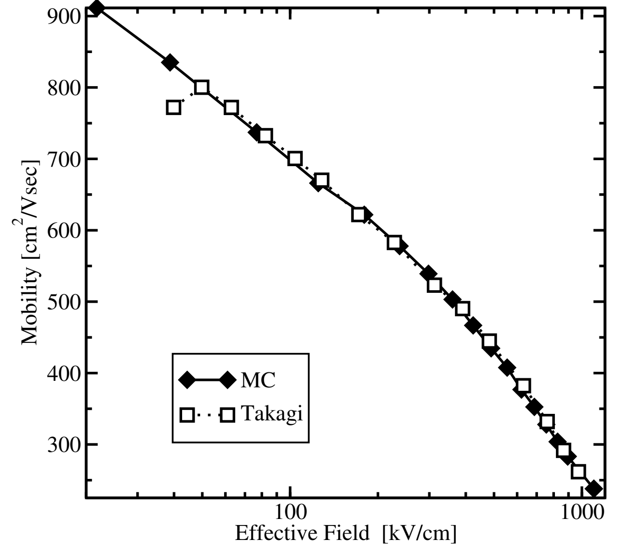

Fig. 3. Comparison of subband MC simulations with the experimental [20] universal mobility of surface layer in silicon. Deviation of experimental mobility from simulations at low effective fields is due to Coulomb scattering not included in MC simulations.

of full-band structure and flexibility of scattering processes of three-dimensional classical MC simulations with the generality of material composition and transport peculiarities due to quantum confinement and strain effects. The MC approach may also be modified to incorporate the quantized character of carrier motion in the direction orthogonal to the current exactly. Although in this case the quantum nature of motion in the confined direction can only be addressed via the solution of the corresponding Schrödinger equation, the carrier motion within each subband may still be considered classical and therefore can be well described by the corresponding Boltzmann equation. Because of possible carrier transitions between different subbands due to scattering, the collision integrals on the right-hand-side of the Boltzmann equation must be augmented with terms describing the intersubband scattering processes. The transport in the inversion layer of ultra-scaled MOSFETs is finally described by the set of Boltzmann equations within each subband, coupled to each other via the intersubband scattering integrals. The set of the subband Boltzmann equations is conveniently solved with the MC methods. This approach therefore combines the advantages of the exact quantum subband description in confinement direction with the classical transport description in transport direction and represents a transition between purely classical and quantum description. An example of the simulation of the low-field surface mobility in inversion layers of silicon, when the transport in the current direction may be treated classically is shown in Fig. 3, together with the experimental "universal mobility" curve [20]. In order to reproduce the universal mobility curve, up to 40 unprimed and 20 primed subbands were taken into account, with realistic electron-phonon and surface roughness scattering included.

III. Quantum-Ballistic Transport

With the aggressive downscaling of MOSFET dimensions continuing, the classical description of carrier motion in transport direction is also gradually loosing its validity. When the characteristic scale of the potential variation along the channel is getting comparable to the carrier De-Broglie wave length, a TCAD model which includes the quantum effects in transport direction must be developed. If dissipative scattering processes can be ignored and particle propagation in the device is coherent, the carrier motion is determined by the solution of the Schrödinger equation, supplemented with open boundary conditions. In order to determine the current density J, it is enough to know the transmission coefficient $TC(\mathcal{E})$ between the source and drain electrodes as well as the supply function $N(\mathcal{E}_x)$ from the electrodes:

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

A similar approach can also be used to determine the gate leakage current [21]. The solution of the Schrödinger equation with open boundary conditions can be achieved by means of the quantum transmitting boundary method [22], [23]. An established alternative framework for these calculations is the non-equilibrium Green's Function method [24] in its reduced coherent version. It is conveniently used for one-dimensional studies of resonant tunneling diodes [25], [26] or carbon nanotubes. 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 [27], [28].

It may appear that in the quantum-ballistic case the knowledge of the full solution of the Schrödinger equation is not necessary and the knowledge of the transmission coefficient is enough for the current calculations. However, the carriers are charged, and their density alters the electrostatic potential in the device via the Poisson equation. The carrier density is proportional to the square of the wave function, so the accurate determination of the transmission coefficient and the current requires a self-consistent solution of the Schrödinger and Poisson equation simultaneously. For quasi-one dimensional transport this can be achieved straightforwardly [29], while the self-consistent solution of the two- or three-dimensional Schrödinger equation together with the Poisson equation represents a computational challenge [27]. Two- and three-dimensional quantum ballistic simulations can be performed by means of an approximate separation of the quantum motion in the confinement direction y from the motion along the current direction x by means of the following ansatz for the wave function $\Psi_n(y,x)$:

$$\Psi(x,y) = \sum_n \xi_n(x)\psi_n(y,x). \quad (4)$$

At discrete positions x, the subband wave functions $\psi_n(y,x)$ are calculated independently from the Schrödinger equation. The transport in the current direction is characterized by the system of one-dimensional Schrödinger equations with open boundary conditions for the wave functions $\xi_n(x)$. Each Schrödinger equation describes the transport inside the particular quantum subband. The quantum transport in each subband is independent from the one in other subbands, if the subband wave functions $\psi_n(y)$ do not depend on the position in x in the transport direction. The Schrödinger equations describing the transport in each subband are decoupled from each other, when the potential $U(x,y)$ in the device is the sum of two contributions, each depending either on y or x coordinate alone. In a general case when the subband wave functions depend on the position x in transport direction, the transport in the subbands n and m is coupled, with the coupling described by the Hamiltonian $\delta H_{nm}(x)$. However, when the intersubband coupling Hamiltonian $\delta H_{nm}(x)$ is small and may be neglected, the transport in the subbands can still be considered as independent from each other. This approximation simplifies the calculations and reduces the computational efforts significantly [30]–[32]. The coupling Hamiltonian is expected to be small if the dependence of the subband wave function on x is weak. An example where the subband decomposition turns out to be an excellent approximation is the ballistic quantum transport in ultra-scaled SOI MOSFETs [32].

The quantum-ballistic description is justified if the size of the channel region is shorter that the phase-breaking length. In carbon nanotubes, where inelastic scattering can be ignored [33], the transport is coherent and therefore well described within the quantum-ballistic approach [5]. An example of the self-consistent simulation for the local density of states, a quantity proportional to the wave function square, is shown in Fig. 4. In silicon MOSFETs, however, the mean-free path at 300 K is only a few nm [34], and the full quantum description which includes dissipative processes must be adopted for MOSFETs with gate length of 10-50 nm. Besides the difficulties of introducing scattering into the simulators based on the coherent description, these simulators are often limited to specific geometries, restrictive grids, or short length scales, which makes their integration into the complex modern engineering TCAD tools problematic. Nevertheless, these simulation approaches are necessary for the estimation of upper bounds of current transport at the quantum limit.

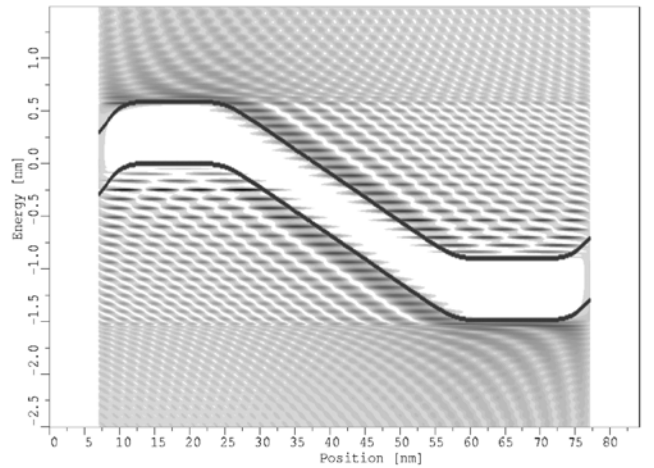

Fig. 4. Local density of states for the carbon nanotube FET as a result of the self-consistent solution of the Poisson equation together with the Schrödinger equation with open boundary conditions [5].

IV. Quantum Dissipative Transport

The methods described so far are either based on the assumption of pure classical or pure quantum nondissipative transport. Nevertheless, in modern microelectronic devices quantum effects are usually dominant in a small active region connected to large, heavily doped contact areas where the carrier dynamics is essentially classical. Therefore, modern TCAD simulators must be able to incorporate both classical and quantum-mechanical modeling. To a certain extent, various quantum corrections can account for the quantum effects, as it was already discussed.

The non-equilibrium Green's functions method addresses the problem in the most consistent and complete way. Due to its completeness, the method is computationally complex and is usually applied to one-dimensional problems [24], for a restricted set of scattering mechanisms [35]. The carbon nanotube FET, which is widely considered to be a potential alternative to the conventional MOSFET, represents an

example where the nonequilibrium Green's function method provides accurate results and is successfully used.

An alternative approach which handles both quantum-mechanical and dissipative scattering effects is based on the Wigner function formalism. Realistic scattering processes can be easily embedded into the Wigner equation via the Boltzmann scattering integral. The Wigner function is given by a transformation of the density matrix [36], [37]

$$f_{\mathrm{w}}(\mathbf{r},\mathbf{k},t) = \int \rho\left(\mathbf{r}+\frac{\mathbf{s}}{2},\mathbf{r}-\frac{\mathbf{s}}{2},t\right)\exp(-\imath\mathbf{k}\cdot\mathbf{s})\,\mathrm{d}\mathbf{s}\ .$$

The kinetic equation for the Wigner function is the Wigner transport equation. It is similar to the Boltzmann equation, with the exception of the extra Wigner potential at the right-hand side:

$$\begin{aligned}\left(\frac{\partial}{\partial t} + \mathbf{v}\cdot\nabla_r + \frac{\mathrm{q}\mathbf{E}}{\hbar}\cdot\nabla_k\right) f_{\mathrm{w}} = \\ \int V_{\mathrm{w}}(\mathbf{r},\mathbf{k}-\mathbf{k}')f_{\mathrm{w}}(\mathbf{k}',\mathbf{r},t)\mathrm{d}\mathbf{k}' + \left(\frac{\partial f_{\mathrm{w}}}{\partial t}\right)_{\mathrm{coll}}\ .\end{aligned} \tag{5}$$

The Wigner potential is defined by

$$\begin{aligned}V_{\mathrm{w}}(\mathbf{r},\mathbf{k}) = &\frac{1}{\imath\hbar\,(2\pi)^3}\int\left(V\left(\mathbf{r}+\frac{\mathbf{s}}{2}\right) - \right.\\ &\left. V\left(\mathbf{r}-\frac{\mathbf{s}}{2}\right)\right)\exp\left(-i\mathbf{k}\cdot\mathbf{s}\right)\,\mathrm{d}\mathbf{s}\ .\end{aligned} \tag{6}$$

Applying the method of moments to this equation, the quantum drift-diffusion [38] [39] and quantum hydrodynamic models [40] [41] can be derived. These models are more convenient for the implementation in conventional 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 is reproduced correctly, the method fails to account properly for tunneling currents [42].

Therefore, a more rigorous approach is desirable to get advantages from both the most accurate classical device simulation approaches and from the quantum-mechanical formulation in Wigner representation. Since the Wigner function formalism treats the scattering and quantum mechanical effects on equal footing through the corresponding scattering integrals, it is attractive to borrow the well established scattering models used in classical MC simulations and solve the quantum Wigner transport equations (5) by means of the MC technique. Such a program was recently realized in [43], [44]. However, since the kernel of the quantum scattering operator is not positively defined, the numerical weight of a particle trajectory increases rapidly, and the numerical stability of a trajectory-based MC algorithm becomes a critical issue. A multiple trajectories method was recently suggested [44] in order to overcome the difficulty. In this algorithm the problem of a growing statistical weight of a single trajectory is addressed by creating an increasing number of trajectories with constant weights, which may assume positive and negative values. Being formally equivalent to the former method, the algorithm

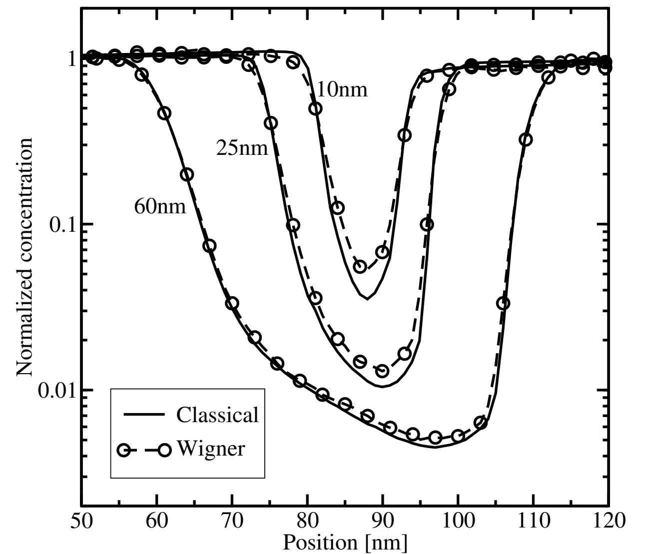

Fig. 5. Comparison of Wigner and classical Monte Carlo results for electron concentration in double-gate MOSFET, for different channel lengths [32].

allows the annihilation of trajectories with similar statistical properties, introducing a possibility to control the number of trajectories. This approach has the advantage that a seamless transition between classical and quantum-mechanical regions in a device is possible [44]. Following [45], one can introduce a spectral decomposition of the potential profile $V(x)$ into a slowly varying, classical component and a rapidly varying, quantum mechanical component. This decomposition is conveniently carried out by applying a low-pass filter with a cut-off wave number $q_c \ll \pi/\Delta x$, where Δx is a grid step size. This separation of the total potential into a classical and a quantum mechanical contribution significantly improves the Wigner Monte Carlo convergence. The method can be applied to the simulation of resonant tunneling diodes [44], and it was recently used for the simulation of 10 nm double-gate MOSFETs [32].

V. Conclusions

Standard classical TCAD tools are gradually loosing their ability to predict accurately the transport properties in the MOSFET devices of a few tenths of nm, their enhancement to meet the engineering demands is needed. A classical six moments model is able to include the hot-carrier effects and reproduce results of the full-band MC, while relevant quantum corrections may be incorporated into different MC schemes. Still the full quantum description is needed for ultra-scaled MOSFETs. Contrary to the carbon nanotubes where the quantum transport is coherent, the quantum dissipative description may be required for transport calculations in ultra-scaled MOSFETs with the gate length as short as 10 nm. The Wigner equation approach is attractive, because it naturally combines the advantages of quantum

descriptions with the accurate scattering models relevant for MOSFETs. However, some constraints for engineering application should be kept in mind. Models must be efficient: Timely results are more valuable than accurate analyses [46]. 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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