Schrödinger Equation Based Quantum Corrections in Drift-Diffusion: A Multiscale Approach

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***Abstract*—In this work, we report the development of a 3D drift-diffusion (DD) simulator for ultrascaled transistors with quantum corrections based on the solution of the Schrödinger equation. In a novel multi-scale simulation approach we use effective masses from tight-binding calculations, carrier mobility from the semi-classical Kubo-Greenwood formalism, and quantum corrections based on self-consistent Poisson-Schrödinger solution. This scheme has been implemented into the University of Glasgow TCAD tool called NESS (Nano Electronic Simulation Software). The approach is validated with respect to non-equilibrium Green's function (NEGF) simulations in the case of nanowire field effect transistors with different cross-sectional shapes.**

Keywords*—*Drift-Diffusion, Quantum-Correction, Kubo-Greenwood, Schrödinger Equation, NEGF, Nanowire FET

I. INTRODUCTION

Numerical transport solvers based on quantum formalisms have very high computational cost and are efficient for the simulation of devices with few nanometers in size. On the other hand, the classical drift-diffusion (DD) approach fails to reproduce the quantum confinement induced shift in the charge distribution in devices with scaled cross-sections like nanowire field effect transistor (NWFETs). A quantum corrected (QC) DD simulator provides a middle ground by ensuring a correct charge profile in the device at reduced computational costs. In this work, in order to facilitate the use of DD formalism to study nanodevices, we have developed and implemented a Poisson-Schrödinger based quantum corrected DD approach while considering the cross-section dependence of the effective masses and the low-field carrier mobilities.

II. SIMULATION METHODOLOGY

Fig. 1 shows the device description and material parameters of a Si GAA NW MOSFET with elliptical cross-section used as an example device for demonstration in this paper. Note that the simulator is capable of handling devices with different geometries, and results for different cross-sectional shapes are discussed later in the paper. Fig. 2 summarizes the approach used in this work that has been integrated into the TCAD tool Nano-Electronic Simulation Software (NESS), developed at the University of Glasgow [1].

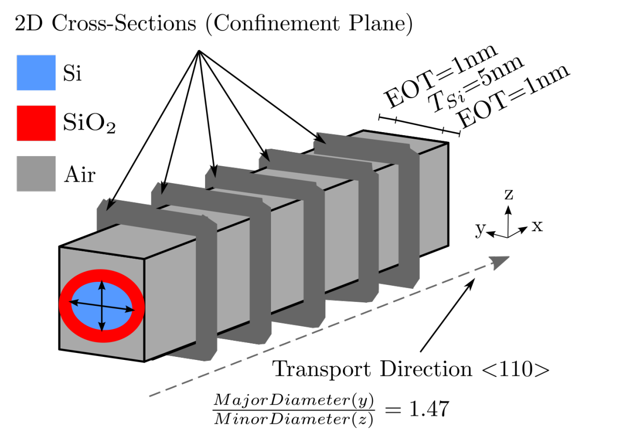


Fig. 1. Sketch of an elliptical nanowire FET. The gate is 10 nm long and it is all-around the intrinsic region. The major and minor axis diameters are 5 nm and 3.4 nm. The transport occurs along the $\langle 110 \rangle$ crystallography direction. The source and drain are highly doped with $N_D = 10^{20}$ cm^{-3}. The oxide layer thickness is 1 nm. The device is at room temperature.

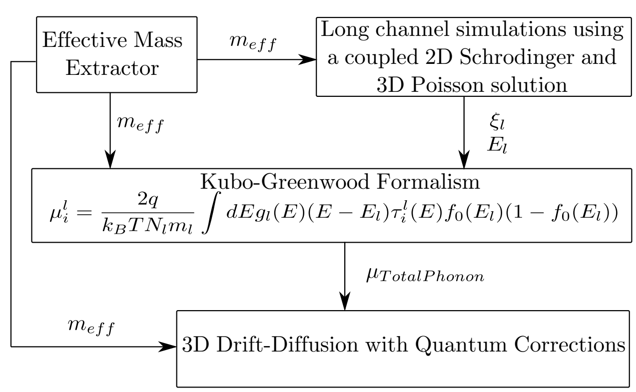


Fig. 2. Scheme showing the flow of the approach proposed in this work. Once the nanowire effective masses are extracted, the low-field mobility is computed by means of the Kubo-Greenwood formalism. The mobility is then input in the DD equations for the charge and current and both are quantum corrected by including the impact of quantum confinement as described in Fig. 3.

As semiconductor devices scale down, it is critical to take into account the dimension dependence of bandstructure and hence effective mass. The effective masses are calculated using full-band structure computed with the QuantumATK atomistic tool [2] andthe effective mass extractor module in NESS [3]. The low-field mobility (which is input to the QC-DD simulator) for the NW is computed by means of the Kubo-Greenwood formalism [4] considering acoustic and optical phonon scattering mechanisms and the long channel approximation [5]. Then, the Matthiessen rule is used to determine the combined effect of the scattering mechanisms [6]. The DD simulator is a 3D tool based on the Scharfetter-Gummel discretization of the drift-diffusion equations using the Bernoulli functions. Different mobility degradation models are also implemented. The Masetti model [7] has been used to capture the effects of doping, Yamaguchi [8] and Caughey-Thomas [9] models have been implemented to take into account the impact of vertical and longitudinal electric fields respectively.

For QC-DD we first solve self-consistently the 2D Schrödinger equation in planes perpendicular to transport and 3D Poisson equation in the whole device. The quantum charge is calculated using a top of the barrier approach [10]. Upon convergence, the resultant 3D quantum charge density is used to calculate a quantum correction term [11], [12]. This term is then used to generate a corrected potential which (instead of the classical potential obtained from Poisson equation) is used as a driving force in the continuity equation. A new quasi-Fermi level is calculated using the corrected potential and charge, which is then fed back to the Poisson's equation in the next iteration as illustrated in Fig. 3. Note that this approach does not use any fitting parameters unlike the density gradient or the effective potential methods.

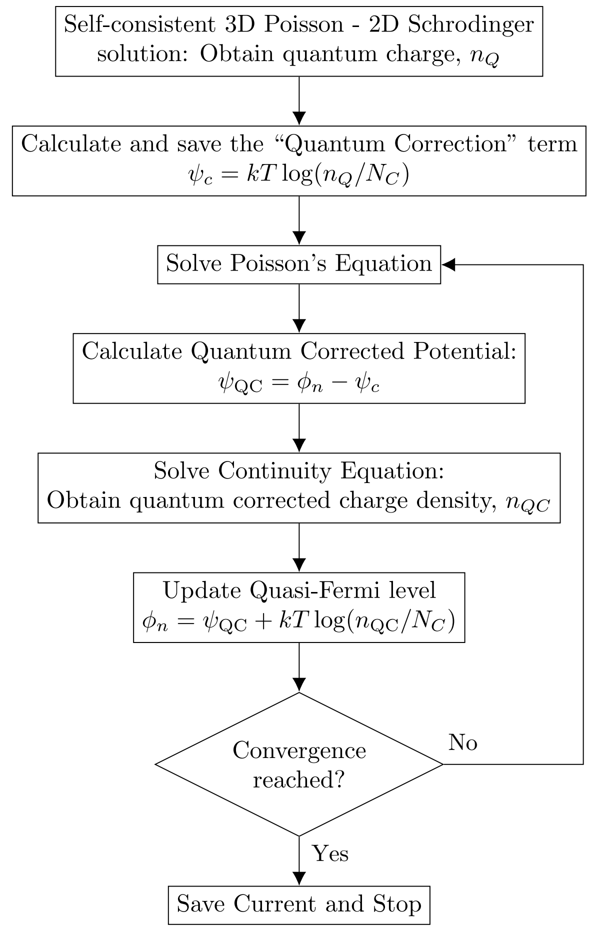


Fig. 3. Flow of the quantum-correction procedure. ψ_c, ψ_{QC}, and ϕ_n are respectively the quantum correction term, the quantum corrected potential, and the quasi-Fermi level. Note that all potential terms have the units of eV in this implementation.

III. Results and Discussion

A. *Comparison of classical DD, QC-DD and NEGF*

Fig. 4 shows the acoustic, optical, and total phonon limited low-field mobilities as a function of the sheet density for the elliptic nanowire. Within the gate bias range considered here, and their corresponding sheet density, the total mobility does not vary much and hence its average value in that range has been used as the effective low-field mobility in the simulations.

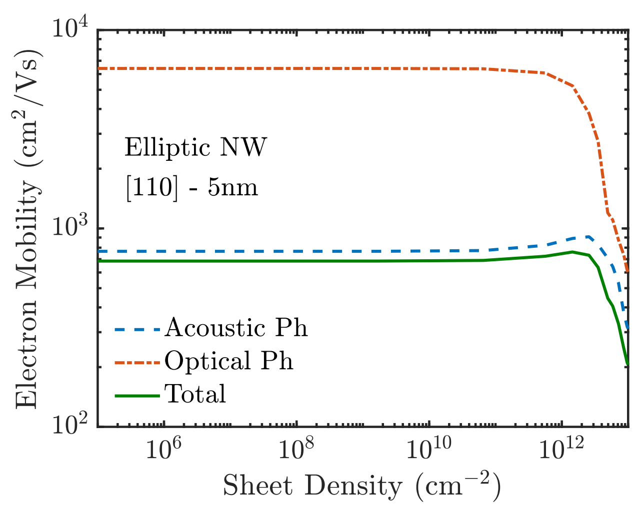


Fig. 4. Acoustic, optical and total low-field mobility as a function of the sheet density for the device in Fig. 1. The total mobility is calculated using the Matthiessen rule.

In Fig. 5 we show a comparison of the 2D charge distribution at the middle of the channel for the three cases: classical DD, QC-DD, and NEGF for V_{GS} = 0.4V, V_{DS} = 0.05V. The quantum nature of the QC-DD charge profile and its close match with the NEGF charge profile is evident.

We compare our current-voltage characteristics with those obtained from the more sophisticated coupled-mode space based NEGF solver in ballistic approximation [13] which is also implemented in NESS [1]. We have used the baseline mobility from Kubo-Greenwood calculations. The results obtained are shown in Fig. 6. Note that treating the mobility as a constant (ignoring its dependence on doping and electric fields) leads to a huge overestimation of the current, and the QC-DD current is much higher than the NEGF current.

On the other hand, using typical parameters for the doping and field dependent mobility degradation models in the QC-DD provides reasonable predictions of the drain current at low drain bias. We obtain very close match with the ballistic NEGF current in the low and medium gate bias regime. At high gate bias, the ballisitic NEGF current exceeds the QC-DD current, as expected. The QC-DD current remains lower than the classical DD current for the entire gate bias range, effectively characterizing the well known threshold voltage shift due to quantum confinement effects.

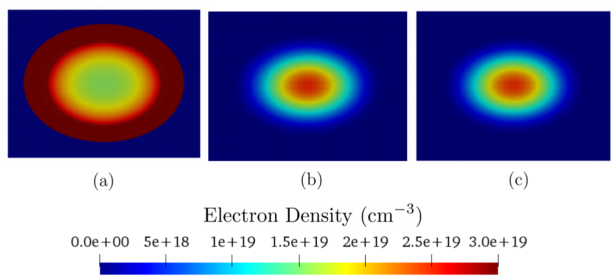


Fig. 5. 2D profile of electron density in the NWFET for (a) Classical DD, (b) QC-DD, and (c) NEGF in the plane normal to transport direction at the middle of the channel. V_{GS} = 0.4 V, V_{DS} = 0.05 V. In case of classical DD, the charge profile is maximum at the edges while for QC-DD and NEGF the maximum occurs at the center. A good match between the QC-DD and NEGF charge distributions is obtained.

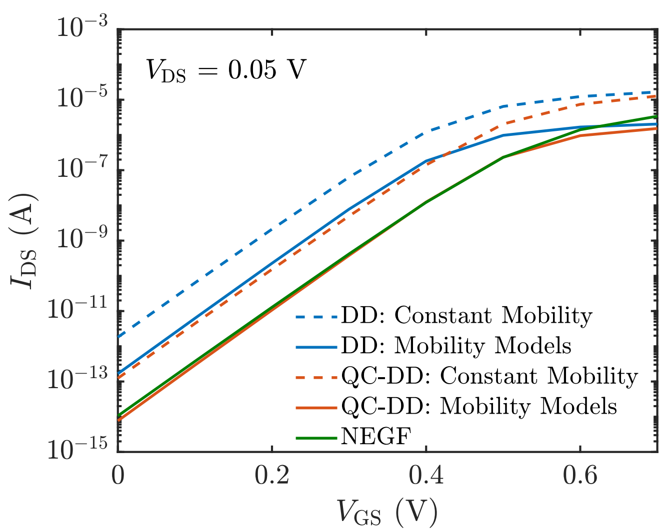


Fig. 6. $I_{\mathrm{DS}} - V_{\mathrm{GS}}$ characteristics computed using classical DD, QC-DD, and NEGF solvers. Using constant mobility results in overestimation of drain current for both DD and QC-DD. When the mobility degradation models are enabled, QC-DD matches very well with the NEGF current especially in weak and moderate inversion. At higher voltages, the QC-DD is noticeably lower than the ballistic NEGF current.

B. Impact of Nanowire Cross-Section Shape

In this section we study the impact of the nanowire cross-section shape using square, circular, and elliptic cross-sections, comparing the DD, QD-DD, and NEGF results. The edge length, diameter, and major axis length of the square, circular, and elliptic NWFET are each 5nm. We follow the same scheme as already described: first the effective masses are evaluated, and then the corresponding mobilities are calculated using the Kubo-Greenwood module. Fig. 7 shows a comparison of the total (acoustic + optical) phonon limited mobilities in the three devices as a function of the sheet charge density. The elliptic cross-section results in the highest mobility, while the circular and square cross-sections yield similar mobilities with the circular one displaying slightly higher values.

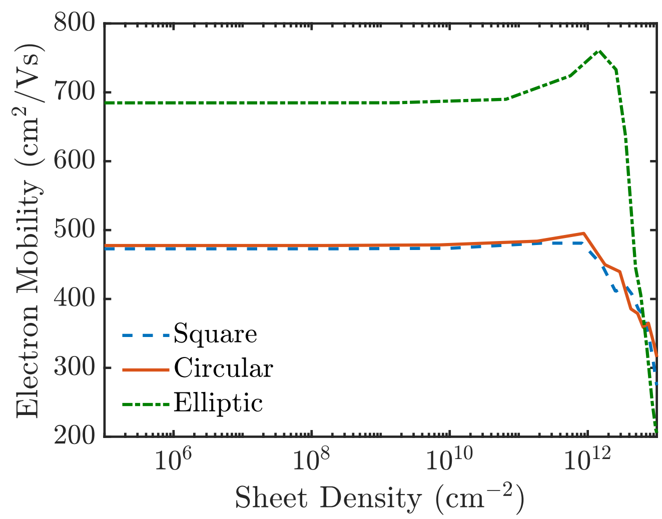
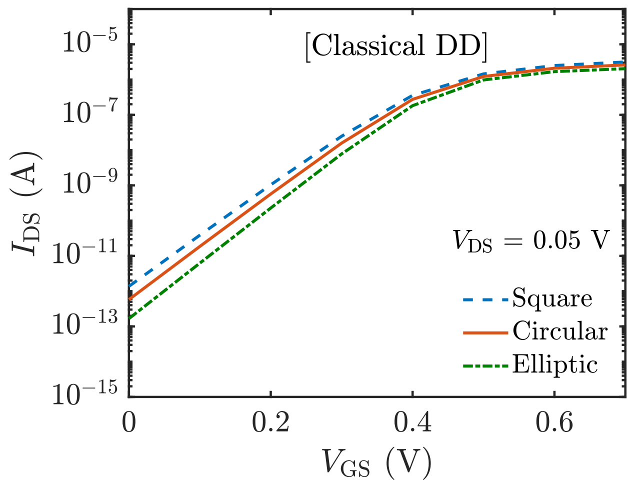


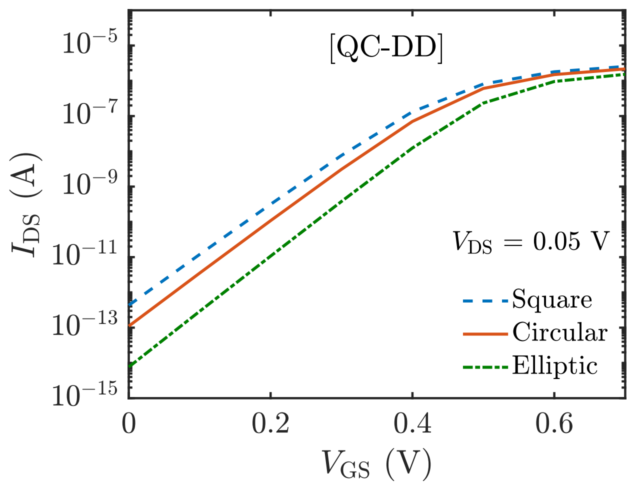
Fig. 7. Comparison of the total (acoustic + optical) phonon limited mobility along ⟨110⟩ direction as a function of the sheet density for different cross-sectional shapes. The elliptic cross-section offers significantly higher mobility.

Finally, we compare the results from the three transport models: classical DD, quantum corrected DD and ballistic NEGF for these three cross-section shapes. There are several interesting observations. First, the nanowire FET with elliptic cross-section delivers the lowest current at all gate biases despite having the highest mobility. All the three transport models are in agreement on this observation. Second, the classical DD, QC-DD and NEGF simulations produce the same trends with regard to the relative performance of the three NWFETs: the square NWFET performs the best in terms of drain current followed by the circular one and then the elliptic one. Third, the magnitude of the impact of the cross-section shape is higher in case of QC-DD and NEGF than the classical DD, as can be seen from the more closely spaced $I_{\mathrm{DS}} - V_{\mathrm{GS}}$ curves in case of the latter. Fourth, the only advantage of the elliptical NWFET is that it offers the steepest subthreshold slope among the three. This is because of the relatively tighter gate control over a portion of the periphery (due to it having a minor axis which is smaller than the diameter of the circular and side of the square nanowire FETs).

This analysis illustrates the pitfalls of classical DD as a direct consequence of not accounting for the quantum confinement effects in highly scaled devices such as the ones examined in this work. It also shows the validity of the quantum-corrected DD to produce results in tune with the NEGF simulations.



(a)



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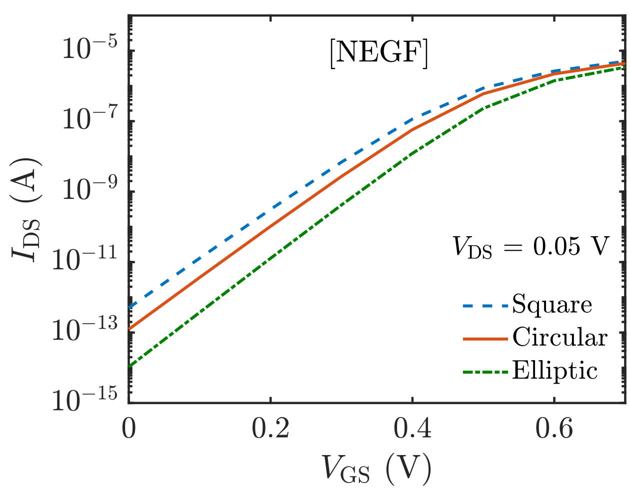

(c)

Fig. 8. Comparison of transfer characteristics of nanowire FETs with different cross-sectional shapes obtained using (a) Classical DD (b) QC-DD (c) NEGF. The elliptic NWFET has the best electrostatics leading to the best subthreshold slope, but lowest current despite having the highest long channel mobility. The square NWFET delivers the highest current. The classical DD fails to properly capture the impact of cross-section shape.

IV. Conclusion

A Poisson-Schrödinger based quantum corrected drift-diffusion simulator has been implemented in our in-house 3D TCAD tool, NESS. The low-field mobility in the GAA nanowire FET is obtained from the 1D multisubband semi-classical module using the Kubo-Greenwood formalism. In addition to ensuring the correct charge profile, the carrier transport includes mobility models that take into account the impact of doping and electric field induced degradation. Our approach shows an excellent agreement in the weak and moderate inversion regimes when compared with NEGF simulations. The impact of different cross-sectional shapes was also studied using the developed models and it was found that a NWFET with square cross-section performs better than one with a circular one while the NWFET with elliptic cross-section fails to translate its high low-field mobility into similar short channel performance although it offers the best electrostatic integrity.

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