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Density Gradient Based Quantum-Corrected 3D Drift-Diffusion Simulator for Nanoscale MOSFETs

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Abstract—In this work, we have developed a solver for the three-dimensional density gradient (DG) equation which is used to apply quantum corrections (QC) to the classical drift-diffusion (DD) simulator in a self-consistent manner. This module has been implemented in C++ using the finite volume method and has been incorporated into NESS (Nano-Electronic Simulation Software) which is being developed in the Device Modelling Group, University of Glasgow. Here, we summarise the implementation details and particularly highlight the impact of the three anisotropic DG masses, which are used as fitting parameters, on the charge profiles and current-voltage (I-V) characteristics in nano-transistors.

Index Terms—Drift-Diffusion; Quantum-Correction; Density Gradient; Quantum Confinement; Nanowire FETs; successive over-relaxation

I. INTRODUCTION

The key motivations for quantum corrected drift-diffusion (DD) simulators are two-fold. First, at nanoscale dimensions, the classical approach cannot reproduce the correct transverse profile of charge density where the charge centroid moves away from the semiconductor/insulator interface due to quantum confinement. Second, the computational cost of full quantum solvers can be prohibitive, particularly when there is a need to perform a large number of simulations, e.g. for statistical variability studies, where a more efficient yet accurate approach is called for. Quantum corrected DD can reproduce the correct transverse profile and the threshold voltage shifts but with much lower computational expense in comparison to quantum solvers.

One way to introduce quantum corrections in DD simulators is using the solution of the Schrödinger equation, which we have implemented in NESS [1]–[6], and has been reported earlier in a previous work [7]. The second approach is using the density gradient (DG) formalism [8], [9] which has been the most widely used quantum correction method to enable the use of drift-diffusion simulators in recent years to correctly model carrier density and transport in nanoscale MOSFETs [10]–[13] with little computational overhead. In this paper, we describe the implementation of a DG equation solver in NESS, and demonstrate the impact of the DG masses.

II. SOLUTION OF THE DG EQUATION

The density gradient formalism involves the introduction of a correction term that is proportional to the divergence of the gradient of the square root of the carrier density, and the DG equation is given by [12], [14]:

$$-\frac{2b_n}{m}\frac{\nabla^2\sqrt{n}}{\sqrt{n}} = \phi_n - \psi - k_B T \ln\left(n/N_C\right), \qquad (1)$$

where n is the carrier density, m is the DG effective mass, ψ is the electron potential energy (eV), ϕ_n is the electron quasi-Fermi level (eV), k_B is the Boltzmann constant, and T is the temperature. $b_n = \hbar^2/4r$, where $\hbar$ is the reduced Planck's constant and r is a dimensionless parameter [14], [15].

In this work we have solved the anisotropic form of the DG equation given by:

$$-\frac{2b_n}{S}\left(\frac{1}{m_x}\frac{\partial^2 S}{\partial x^2} + \frac{1}{m_y}\frac{\partial^2 S}{\partial y^2} + \frac{1}{m_z}\frac{\partial^2 S}{\partial z^2}\right)$$
$$= \phi_n - \psi - k_B T \ln\left(S^2/N_C\right), \qquad (2)$$

where $S = \sqrt{n}$, (m_x, m_y, m_z) are the anisotropic DG effective masses in the three directions, and in this work $r=3$ has been used. The equation is solved for S.

The solution method for DG equation is analogous to that of the non-linear Poisson's equation. The DG equation is integrated over volume, divergence theorem is applied on the left hand side, and then discretized using the finite-volume approach. We have applied successive over-relaxation approach with Chebyshev acceleration for the solution along with red-black parallelism. More details can be found in the NESS manual [1]. At Source/Drain Contacts, Neumann type boundary condition is applied on carrier density. At present, at the Si/SiO$_2$ interface, the boundary condition on S is fixed to low value to effectively make the carrier density vanish there assuming infinite barrier [12]. It can be modified to consider smooth penetration into the oxide. The corrected carrier density and potential both float at S/D contacts.

III. DG CORRECTION PROCEDURE

The left hand side of (2) is the "density gradient" correction to be applied to the classical potential. The quantum corrected potential is:

$$\psi_{qc} = \psi - \frac{2b_n}{S}\left(\frac{1}{m_x}\frac{\partial^2 S}{\partial x^2} + \frac{1}{m_y}\frac{\partial^2 S}{\partial y^2} + \frac{1}{m_z}\frac{\partial^2 S}{\partial z^2}\right). \quad (3)$$

This can be equivalently re-written using (1) as:

$$\psi_{qc} = \phi_n - k_B T \ln\left(S^2/N_C\right). \quad (4)$$

Thus, in essence, the solution of the DG equation is used to calculate a quantum correction term, $\psi_q = k_B T \ln(S^2/N_C)$, which is then used to generate the quantum corrected potential as: $\psi_{qc} = \phi_n - \psi_q$. Instead of the regular Gummel iterations where only Poisson and current continuity equations are solved self-consistently, in DG corrected DD, after Poisson solution, the DG equation is solved as well in order to generate the correction term. The quantum corrected potential is then used as the driving force while solving the current continuity equation to yield a quantum corrected charge density, and finally current is evaluated. Note that while solving the DG equation, the quasi-Fermi level ($\phi_n = \psi + k_B T \ln(n/N_C)$) remains fixed to the value obtained after the solution of the current continuity equation in the previous Gummel iteration. The full procedure is summarised in the flowchart in Fig. 1.

Solve Poisson's Equation

Solve DG Equation:
Obtain DG carrier density: $n_{\mathrm{DG}} = S^2$

Calculate the Quantum Correction term
$\psi_q = k_B T \ln(S^2/N_C)$

Calculate Quantum Corrected Potential:
$\psi_{qc} = \phi_n - \psi_q$

Solve Continuity Equation
Obtain quantum corrected carrier density
Evaluate Current

Convergence reached?   No
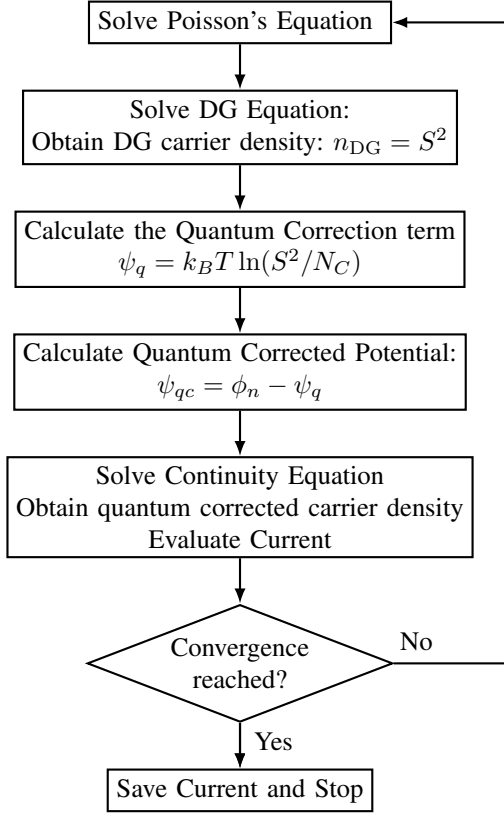
Yes

Save Current and Stop

Fig. 1. Density gradient based correction to drift-diffusion is implemented as a self-consistent solution of the Poisson, density gradient, and current continuity equations.
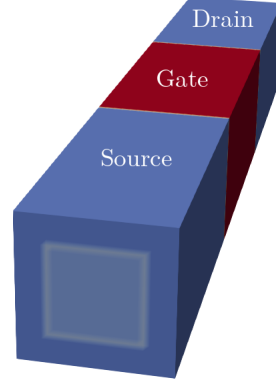

Fig. 2. Nanowire FET structure simulated in this work as an example. The cross-section is square shaped with edge length, t_{Si}=3nm; gate length, L_g=10nm; Source/Drain length, $L_{S/D}$=10nm; oxide thickness, t_{ox}=1nm.

IV. IMPACT OF THE DG EFFECTIVE MASSES

In this section, we analyse the impact of the DG effective masses on the carrier distribution and the current-voltage characteristics in nano-transistors. As an example, a silicon nanowire field effect transistor (NWFET) with 3nm × 3nm square cross-section, and gate length of 10nm as shown in Fig. 2 has been simulated.
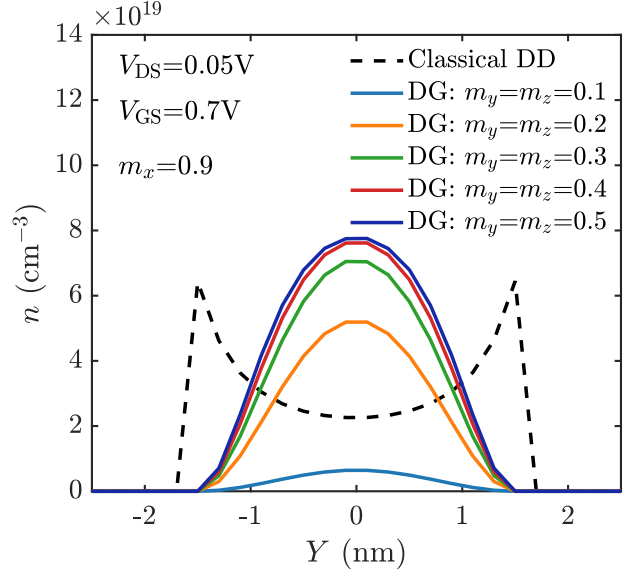
A. Transverse DG Effective Masses

Fig. 3. Effect of varying the transverse DG effective masses on the electron concentration along the transverse direction at the middle of the NWFET channel, at fixed longitudinal DG effective mass of $0.9m_0$. The classical DD result is included for comparison.

The DG effective masses in the transverse direction, m_y and m_z, prominently affect the quantum confinement in the device. We varied m_y and m_z simultaneously keeping them equal while the longitudinal effective mass, m_x was fixed to

0.9m_0. The results are shown in Fig. 3. It is clear that the DG approach can capture the quantum confinement effects and the carrier distribution peaks at the center of the NWFET, in contrast to the classical DD case where the peak is at the Si/SiO$_2$ interfaces. Also, it is seen that the peak value of the carrier distribution increases with increase in the value of the transverse effective masses.

Further, in Fig. 4, we have shown the transfer (I_D-V_G) characteristics of the NWFET for the different transfer DG masses. As expected, lower transverse effective masses lead to increased confinement effects and hence larger threshold voltage (V_t) shift. This is similar to the effect of reduced effective masses in a quantum treatment of the electrostatics and transport as seen in Poisson-Schrödinger or NEGF based simulations. The amount of V_t shift tends to saturate as the transverse effective masses are increased.
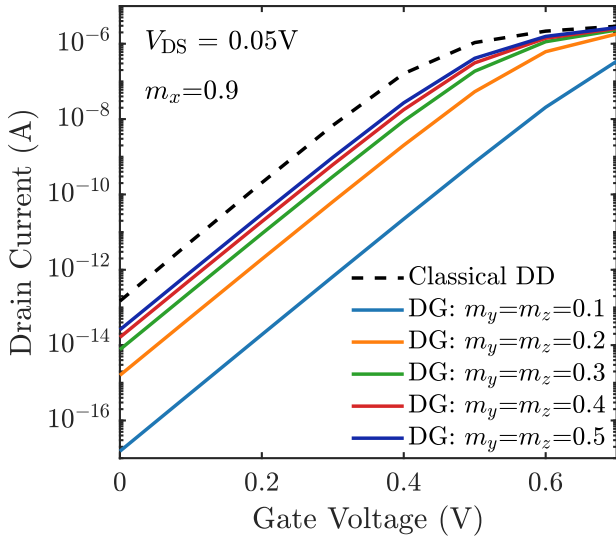

Fig. 4. Impact of transverse DG effective masses on the $I_D - V_G$ characteristics of the NWFET. Compared to classical DD, the DG corrected DD I-V curves display a threshold voltage shift, with the shift being higher for lower transverse masses.

B. Longitudinal DG Effective Mass

The impact of the longitudinal effective mass (m_x) on carrier distribution at the center of the device along the transverse direction at fixed values of the transverse effective masses is shown in Fig. 5 at low and high gate biases. It can be observed that at high gate bias (V_G=0.7V), there is little dependence of the magnitude of carrier concentration on m_x unlike the transverse DG masses. However, at low gate bias (V_G=0V) i.e. in subthreshold, a smaller m_x leads to higher peak electron concentration. This is also reflected in a smaller m_x resulting in an increase in the subthreshold slope and off-state leakage as illustrated in Fig. 6. This effect of degraded subthreshold characteristics at lower m_x is similar to what is obtained from full quantum transport simulation in nano-transistors as the effective mass of the channel material in the transport direction is reduced and is attributed to direct source-to-drain tunneling [16], [17]. Hence, this impact of m_x can be

used to calibrate the subthreshold slope and thus the impact of source-to-drain tunneling as well in scaled devices.
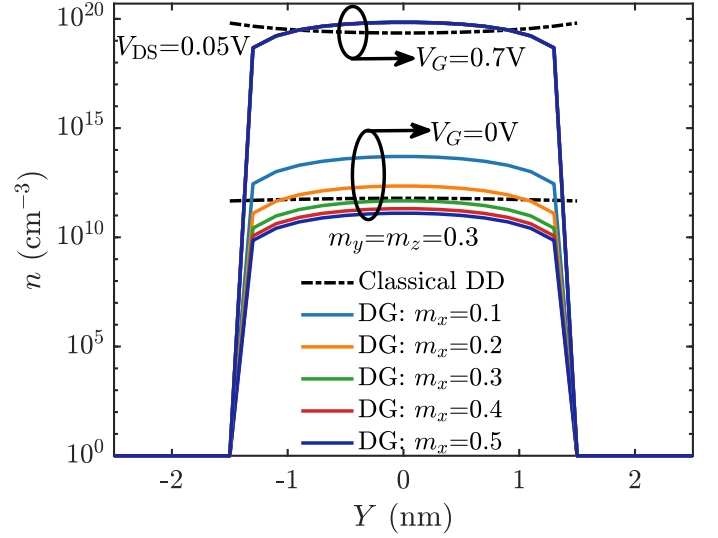

Fig. 5. Effect of varying the longitudinal DG effective masses on the electron concentration along the transverse direction at the middle of the NWFET channel, at fixed transverse DG effective masses, both m_y and m_z being set to 0.3m_0. The behavior is markedly different at low and high gate bias conditions. The classical DD result is included for comparison.
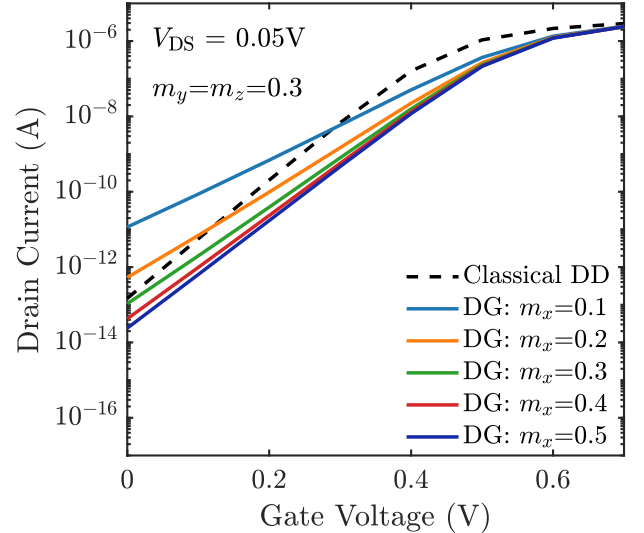

Fig. 6. Effect of varying the longitudinal DG effective mass (m_x) on the transfer characteristics of the NWFET. Smaller m_x leads to worsening of the subthreshold slope and increase in off-current.

V. CONCLUSION

In this paper we have described the density gradient approach of introducing quantum corrections to a classical three-dimensional drift-diffusion simulator using the anisotropic density gradient formalism. We have elucidated the effects of the three DG effective masses on the carrier density profiles and current-voltage characteristics in a nanowire transistor.

These results demonstrating the different behaviour of the DG effective masses which are used as fitting parameters, will be useful while calibrating the DG corrected DD simulator against results obtained from more sophisticated transport simulations e.g. using the NEGF formalism.

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