Comparison of Density Gradient and NEGF for 3D Simulation of a Nanowire MOSFET

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Abstract—The density gradient quantum correction to the conventional drift-diffusion simulation technique has become a well established method to include quantum mechanical effects without resorting to a full quantum transport solution. The results obtained from this method, however, can depend greatly on the values of certain parameters used, and it is usual to calibrate the simulation against more rigorous quantum transport simulations such as non-equilibrium Green’s functions (NEGF). Here we present an analysis of the effect of varying fitting parameters within density gradient and compare the results to NEGF simulations for a nanowire transistor.

I. INTRODUCTION

As device dimensions shrink to the order of nanometres, quantum effects such as confinement and tunnelling start to play a significant role. Quantum confinement shifts the threshold voltage, and the leakage increases due to band-to-band, source-to-drain and gate tunnelling. Such effects will have a strong impact on the performance of nanowire transistors actively researched at present as a possible replacement for bulk, Ultra-Thick Body (UTB) SOI and Multi-Gate (MG) MOSFETs near the end of the roadmap. At the same time, it is expected that nanowire MOSFETs will suffer from strong variability problems since a single stray dopant or atomic scale interface roughness could have a dramatic effect on the device characteristics at small nanowire cross-sections [1]. 3D quantum transport simulators based, among others, on the Non-Equilibrium Green’s Function (NEGF) formalism, are the best vehicles for studying quantum effects in nanowire transistors [2,3]. However they are computationally expensive and when simulation of variability on a statistical scale has to be carried out, more economical quantum correction techniques have to be used [4]. Thus, such techniques have to be thoroughly compared, calibrated and validated with respect to full scale quantum transport simulators to ensure physically meaningful and reliable results.

At the same time, one of the most successful techniques to simulate electronic devices has been the Drift-Diffusion (DD) approach which essentially is a low order approximation to the Boltzmann transport equation. The DD method can be modified to account for quantum mechanical effects by means of quantum correction techniques. One straightforward, and widely accepted, quantum correction is the density gradient (DG) approach [5]. It mimics the quantum repulsion of the electrons from the surface of a confining potential by introducing an effective quantum potential, which is dependent on the gradient of the electron density.

Here, in direct comparison with NEGF simulations, we investigate the influence and the optimal adjustment of the effective masses used as fitting parameters within the density gradient method, and the range of validity and accuracy of the DG approach.

II. SIMULATION TECHNIQUE

A. Density Gradient – Drift Diffusion simulation

For the solution of the density gradient corrected drift-diffusion approximation we use a modified Gummel approach [6] where the Poisson equation (1) and Density Gradient equation (2), for a given electron Fermi-level distribution, are solved self-consistently for the electrostatic potential and the quantum-corrected electron density.

\[
\nabla \cdot (\varepsilon \nabla \psi) = -q \left( p - n + N_D^* - N_A^* \right) \quad (1)
\]

\[
\frac{2b_n^2}{S} \left( \frac{1}{m_e} \frac{\partial^2 S}{\partial x^2} + \frac{1}{m_i} \frac{\partial^2 S}{\partial y^2} + \frac{1}{m_i} \frac{\partial^2 S}{\partial z^2} \right) = \phi_n - \psi + \frac{k_B T}{q} \ln \left( \frac{S^2}{S_0^2} \right) \quad (2)
\]

where \( S = \frac{n}{n_i} \) and \( b_n^2 = h^2/4 q r \). Equation (2) is the anisotropic density gradient equation [7] so there are different effective mass components in the transport (longitudinal)
direction, \( m_x \) from in the confinement (transverse) directions, \( m_y \) and \( m_z \). These effective masses are treated as fitting parameters.

The effective quantum-corrected potential is then calculated from:

\[
\psi_{\text{eff}} = \psi + \frac{2\hbar}{S} \left( \frac{1}{m_x} \frac{\partial^2 S}{\partial x^2} + \frac{1}{m_y} \frac{\partial^2 S}{\partial y^2} + \frac{1}{m_z} \frac{\partial^2 S}{\partial z^2} \right) = \phi_n + \frac{k_B T}{q} \ln(S^2)
\]

and is then used as the driving potential for the current continuity equation:

\[
\nabla \cdot J_n = 0
\]

where

\[
J_n = -q\mu_n \nabla \psi_{\text{eff}} + qD_n \nabla n
\]

which is solved using a standard Sharfetter-Gummel discretisation based on the effective quantum-corrected potential. The system of equations (1&2) and (4) are solved self-consistently until convergence.

In the NEGF approach, Neumann boundary conditions (NBC) are used in the source and drain, as the potential adjusts to preserve charge neutrality. We have also implemented such NBC in the density gradient simulator [8], rather than the usual Dirichlet boundary conditions (DBC) for the ohmic source/drain contacts used in DD simulations. The NBC work better in conjunction with the density gradient in the sense that they do not restrict the potential and electron concentration in the source and drain from following the distribution imposed by quantum mechanics. The Si/SiO\(_2\) boundary conditions for the quantum potential in the density gradient approach require careful consideration, and in our simulations we use the approach of Jin, et al [9]. This method fixes the gradient of the electron concentration perpendicular to the Si/SiO\(_2\) interface depending in the relative effective masses in the silicon and the SiO\(_2\), accounting for penetration of the electron wave function into the oxide.

### B. Non-Equilibrium Green’s function simulation

We have used a fully self-consistent 3D real space NEGF simulator [1] in the effective mass approximation. The NEGF formalism is essentially based on two equations. The first one describes the propagation of a single electron through the device [10].

\[
G^R = (E-H+\Sigma^R)^{-1}
\]

where \( G^R \) is the retarded Green function or propagator. The superscript \( R \) indicates the boundary condition for the electron propagation (i.e. that the Fourier transform of this propagator (\( G \)) will not transport an electron from the future to the past). Here, \( E \) is the total energy of the electron; \( H \) is the Hamiltonian, which contains the kinetic plus the potential energy of the electrons; \( \Sigma^R \) is the contribution to the energy of the electron due to the coupling to the contacts and other

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Fig. 2. \( I_D-V_G \) characteristics showing the effect of varying \( m_x \) (\( m_y=m_z=0.12 \)). A comparison with NEGF is shown.

Fig. 3. \( I_D-V_G \) characteristics showing the effect of varying \( m_y \) and \( m_z \) (\( m_x=0.8 \)). A comparison with NEGF is shown.

Fig. 4. Electron concentration along the centre of the nanowire varying \( m_x \) (\( m_y=m_z=0.12 \)).

Fig. 5. Electron concentration across the middle of the nanowire varying \( m_x \) (\( m_y=m_z=0.12 \)).
effects such as phonons. $\Sigma^R$ contains the information about the retarded boundary condition.

The second equation is a statistical equation which controls the local movement of electrons in and out of a particular energy state leading to the $G^-$ propagator \[ G^- = G^R \Sigma^- G^{R+} \] (7)

Here the ‘+’ represents the hermitian conjugate, and $\Sigma^-$ is the statistical scattering matrix. This equation becomes a straightforward expression for calculating $G^-$ when there are no processes which redistribute the energy of the electrons. In the general case the $\Sigma^R$ will depend on $G^-$, and (6) and (7) need to be solved self-consistently. In our model the Hamiltonian is written in the effective mass approximation.

### III. RESULTS AND DISCUSSION

#### A. Continuous channel doping

Here we investigate the effect on $I_D-V_G$ curves and on electron density of varying the effective mass parameters and compare the results to fully-3D NEGF simulations. Fig 1 shows a schematic diagram of the simulated wrap-around-gate nanowire that we simulate for this investigation.

Fig 2 shows that the effect of reducing $m_z$ is to drastically change the subthreshold slope. In order to closely match the slope obtained from the NEGF simulations a longitudinal mass between 0.5$m_0$ and 0.8$m_0$ would be required in this case. This is significantly larger than the transverse mass that is usually needed to account for quantum confinement. If an isotropic mass were used, it is likely that the value would be chosen to match the desired confinement characteristics resulting in a mass which could seriously degrade the subthreshold slope when density gradient is applied.

In the case of the wrap-around-gate nanowire MOSFET studied here, both of the transverse masses, $m_x, m_y$, control the confinement in their respective directions and are kept equal in the presented simulations. Fig 3 shows that changing $m_x, m_y$ changes the threshold voltage shift due to a change in confinement. If these masses are large then the effect of the quantum correction is small and the results are closer to those obtained from a classical simulation. Reducing the transverse masses increases the effect of the quantum correction resulting in carriers being pushed further away from the interfaces and inducing larger threshold voltage shift.

Figs 4-7 illustrate the effect on the electron distribution of changing the different masses. Fig. 2 indicates that reducing $m_z$ increased the subthreshold current. Figs 4 and 5 show that there is an associated increase in the electron concentration in the channel of the device. It is clear that it is possible to match quite closely the electron distribution obtained from NEGF simulations, however the value of $m_z$ required in order to do so ($m_z=0.1$) is very low for the longitudinal mass when one considers the effect on subthreshold slope of small masses which was observed in Fig. 2. Fig. 5 also demonstrates that
changing $m_z$ does not affect the shape of the electron distribution in the transverse directions.

Figs 8 and 9 show that if density gradient is calibrated to NEGF at a particular gate voltage then that agreement can hold over a range of gate voltages. Matching the electron distribution of NEGF, however, again suggests a value of $m_z$ that is lower than that used to match the $I_D-V_G$ characteristics, which could result in degradation of the subthreshold slope.

B. Discrete dopant in the channel

While the channel of the nanowire MOSFET is nominally undoped, in reality it is possible that localised charges may exist, associated with stray dopants or trapped carriers. It is important to resolve the impact of these stray charges on the device characteristics. We look at how well the DG simulations can match the NEGF simulations when a stray discrete dopant (donor) is introduced in the middle of the channel. Fig 10 shows how well the electron distributions can match for a range of gate voltages. Using the same parameters as for the case with no dopant, the $I_D-V_G$ characteristic with a dopant included also agrees very well with the NEFG simulation.

It is clear that in the presence of localised charges the density gradient can be calibrated to produce excellent agreement with NEGF for either the carrier distribution or the $I-V$ characteristics. Unfortunately the values of the effective mass parameters required to match the NEFG simulations are different between the two cases.

IV. CONCLUSIONS

We have presented an investigation of the dependence of $I-V$ characteristics and electron distributions on the values chosen for the effective masses which are used as fitting parameters in the density gradient method. This was done in comparison with the results of non-equilibrium Green’s function simulations. We find that it is possible to match the threshold voltage shift and subthreshold slope of the simulated I-V characteristics, and also the electron distribution within the device over a range of gate voltages. However, a different set of effective mass parameters are required in each case. In general, transverse masses $m_y=m_z=0.1-0.2$ are required in all cases, however the longitudinal mass requires a large value, $m_z=0.8$, to prevent an undesirable swing in the subthreshold slope, while a small value, $m_z=0.1$, is required to closely match the electron distribution along the channel. It is clear that these parameters much be chosen carefully depending on the priorities of particular simulations.

REFERENCES