Development of a Full 3D NEGF Nano-CMOS Simulator

A. Martinez, J. R. Barker , A. Asenov
Dept. of Electronic and Electrical Engineering
University of Glasgow
Glasgow, UK
antonio@elec.gla.ac.uk

M. Bescond
IMEP-ENSPG
Rue des Martyrs, Cedex1
Grenoble, France

A. Svizhenko
Dept. of Mechanical Engineering
Stanford University
McCullough bldg
California, USA

A. Anantram
Electrical and Computer Eng. Dept,
University of Waterloo
Canada

Abstract— **We describe the development of a new fully 3D NEGF simulator. At this stage we illustrate the use of the corresponding 3D NEGF solver to study, non-self consistently, the effect of the spatial inhomogeneities caused by stray charges and rough Si/SiO2 interface in nano-CMOS devices. These cannot be accurately described using perturbative techniques. The use of decoupled simulations is justifiable in the subthreshold region of device operation. In the presence of the above imperfections the current and charge density have a distinct 3D character.**

Keywords: Non Equillibrium Green Function, Nanotransistor , three dimentional quantum simulations, unintentional dopants

I. INTRODUCTION

Quantum mechanical confinement and tunneling profoundly affect the performance and the leakage of the present and next generation nano-CMOS devices. The techniques, used in the simulation of such effects, range from relatively simple quantum corrections introduced in drift-diffusion and Monte Carlo simulators to the development of full scale quantum transport simulators based on the solution of the Schrödinger equation [1], Wigner function equation [2] and the Non Equilibrium Green's Function (NEGF) formalism [3]. In recent years the NEGF approach has gained significant momentum and has become the preferred choice in the development of quantum transport simulators and in the study of the behavior of nano-CMOS devices, with novel device architectures and novel channel materials. Yet most of the existing NEGF simulators are based on the mode-space approach coupling the 1D NEGF solution in the direction of the transport to 1D [4] or 2D [5] solution of the Schrödinger equation in the normal to the transport direction device cross-section. Although computationally efficient, such an approach cannot be used to realistically study the impact of different sources of intrinsic parameter fluctuations in nano-CMOS transistors. Such sources include random discrete dopants, interface roughness, body thickness fluctuations and LER resulting in a non-homogeneous flow and multiple current percolation paths in the corresponding devices.

For example the atomic scale steps at the Si/SiO2 interface in conjunction with the thermal wavelength of an electron, which is in the order of nanometer, implies that the interaction between electron and the unique interface roughness pattern in the nano-CMOS devices needs to be treated quantum mechanically. The same is true for stray charges localized in the active region of such devices. Previously we have used 2D NEGF simulations to illustrate qualitatively the impact of such sources of intrinsic parameter fluctuations on the behaviour of ballistic devices [1]. They however use 1D representation of interface roughness and wire-like localised charges, which can completely block the current flow in thin body devices, resulting in an overestimation of the corresponding fluctuations.

In this paper we describe the development of a full 3D NEGF simulator, which will be used to study highly inhomogeneous transport in nano-CMOS devices with complex geometry and in the presence of different sources of intrinsic parameter fluctuations. We also illustrate the essential features of the 3D NEGF solution in a set of non-self consistent examples showing the impact of stray impurities in the channel of nanowire MOSFETs on the 3D electron current and density.

II. THE 3D GREEN FUNCTION SIMULATOR

The NEGF approach allows the computation of the amplitude of probability for an electron with an energy E to go from a point $\boldsymbol{x}$ to a point $\boldsymbol{y}$ in the real space, i.e. the propagator $G^r(\boldsymbol{x}, \boldsymbol{y}, E)$. This is essentially the inverse of the matrix formed by the Hamiltonian minus the energy of the electron. In the absence of a scattering, the correlation matrix $F(\boldsymbol{x}, \boldsymbol{y}, E)$ can be computed as

$$F = G^r \Omega G^a \tag{1}$$

Where G^a represents the Hermitian conjugate of G^r. Ω is the statistically weighted self-energy proportional to the Fermi-Dirac function and the inverse of the electron lifetime in the device (i.e. the lead-device coupling energy). The diagonal elements of F are proportional to the electron density and the off diagonal elements can be used to calculate the current density. The electrons are injected from the source and drain following the Fermi-Dirac distribution. The fact that the NEGF formalism follows the motion of an electron at a fixed energy makes this technique particularly simple when treating transmission problems and ballistic transport compared to other techniques like the Wigner function formalism which mix position and momentum state representations and might be better suited to treat inelastic processes.

The 3D NEGF simulator described here solves the matrix form of Eq. 1 in order to compute the current and electron density. At this stage the potential distribution is obtained from the non-self consistent 3D solution of the Poisson equations, which reflects the device geometry and the bias applied at the terminals. The Coulomb potential of unscreened individual stray dopants is added to the Poisson solution. The Hamiltonian is in effective mass Hamiltonian approximation. The well known computational and memory intensity of the 3D NEGF formalism requires the use of efficient algorithms that avoid the need to compute the inverse of the full 3D Hamiltonian. A recursive algorithm [3] allows us to compute just the diagonal and off-diagonal elements of the inverse matrix following Dyson's equations. The self-energies for the contacts are calculated following the approach described in [6]. The simulator allows the use of different boundary conditions (zero value or periodical) for the wave function at one pair of boundaries in a direction perpendicular to the channel of the device.

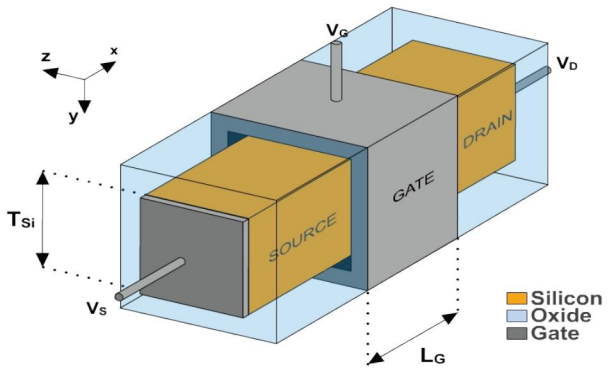

Figure. 1 The geometry and co-ordinated system of (gate all around) nanowire MOSFET

III. RESULTS

The 3D NEGF approach is illustrated in the simulation of a nanowire MOSFET, the geometry and co-ordinate system of which is presented in Fig. 1 This undoped channel transistor has 6 nm channel length, 2×2 nm channel cross-section, 1 nm thick gate oxide and 10^{20} cm^{-3} doping concentration in the source/drain regions. Fig. 2 illustrates the potential distribution in the at z =2 nm (x,y) plane at V_G=0.3 V and V_D=0.2 V for a uniform device without unintentional dopant and rough surface. Note that the potential in the source/drain varies in the y direction because the wave function of the electron is set to zero at the interface but the doping concentration is assumed constant in source/drain regions.

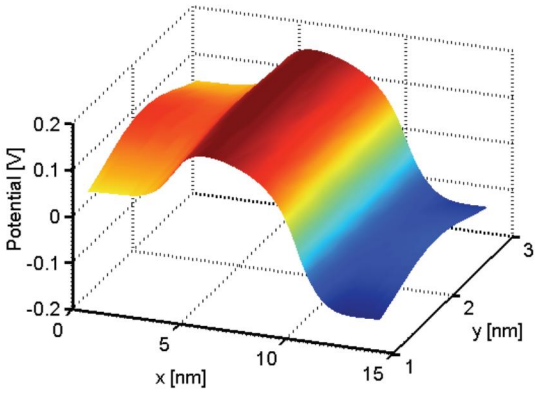

Figure 2 Potential profile in the plane z=2 nm along the channel at V_D=0.2 V

Fig. 3 shows the electron concentration distribution in the same plane. The electron concentration goes to zero at the interface due to the afore-mentioned boundary condition for electron wave function.

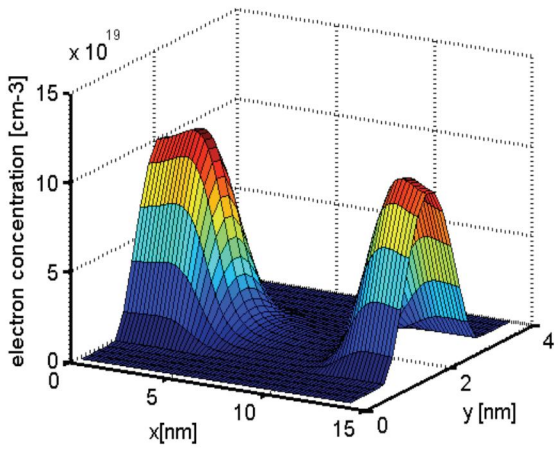

Figure. 3 Electron density for the same plane and potential as Fig. 2.

The upper panel of Fig. 4 shows the potential distribution in the y =2.6 nm (x,z) plane along the channel of a transistor with a single stray donor located in the (6, 2.6, 2.0) position. The lower panel in the same figure shows the distribution of the x component of the current vector J_x in the same plane. It is clear that J_x is not conserved in this plane because the current has a component perpendicular to the channel direction. In a 2D analogue of this case the current will be practically blocked by the stray donor but in the 3D case the current can flow around it. Note also that there is very little tunneling through the impurity i.e. the current is almost zero at the impurity position.

Fig. 5 shows the potential and the current density in the same device but in the z=2 nm (x,y) plane.

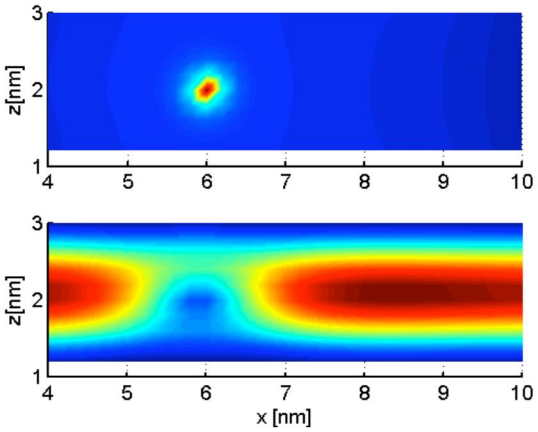

Figure 4 The potential (Upper panel) and current density (Lower panel) at the plane y=2.6 nm for a device with an impurity located in (6, 2.6, 2.0) nm

In this plane the position of the impurity is closer to the oxide interface producing a mild disturbance in the current flow. The current meanders around the impurity position contrary to the case of fig. 4 in which the current is almost totally blocked due to the combined effects of the boundary condition pushing the electron to the center of the plane and the impurity potential barrier blocking the passage of the electron in that plane.

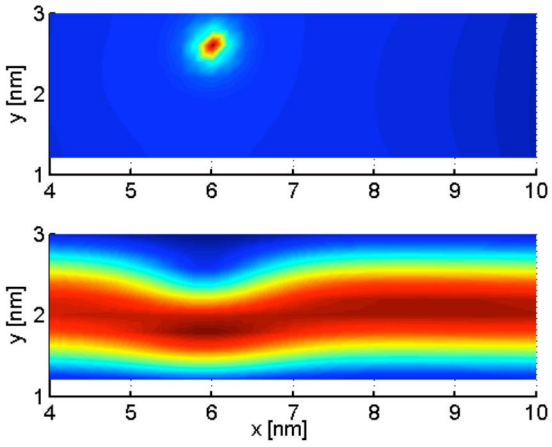

Figure 5 The potential (Upper panel) and current density (Lower panel) at the plane z=2.0 nm for the same device as Fig. 4.

The electron density in a cross section normal to the channel containing the impurity is shown in fig. 6. Note the distortion in the electron density due to the impurity location. This reflects the distortion of the transversal wave function, which extends over 1 nm. This transversal state has a considerably higher energy when compared to the transversal state, without the impurity, because of the additional confinement introduce by the impurity potential.

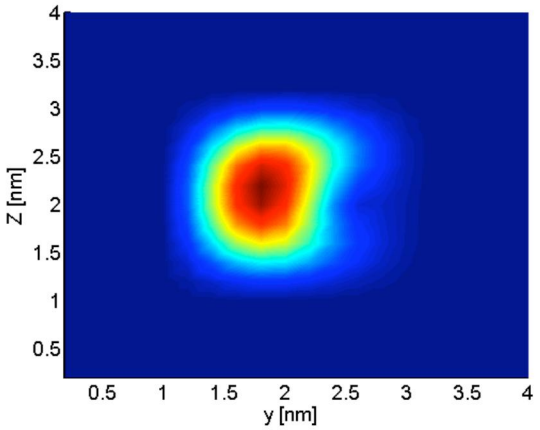

Figure 6 The distorted electron density in the plane x=7.5 nm, at the impurity location. The distortion extended around 1nm along the channel.

Finally, we have computed the electron and current density for two non-aligned (negatively charged) repulsive impurities in the channel, in order to illustrate more complex situations. In the present case the impurities are located in the same y-plane but in different z-planes

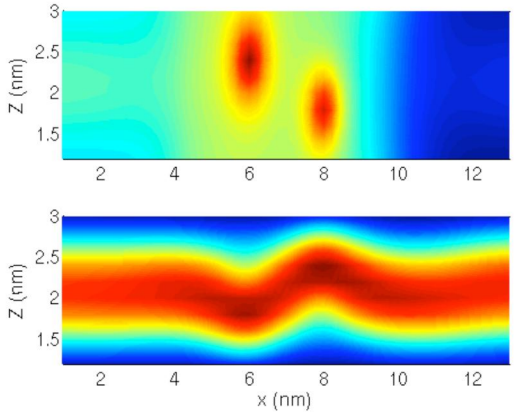

Figure 7 The potential (Upper panel) and current density (Lower panel) at the plane y=2.0 nm for a device with two non aligned impurities located at (6, 2.4, 2.4) nm and (8,2.4,2.0) nm

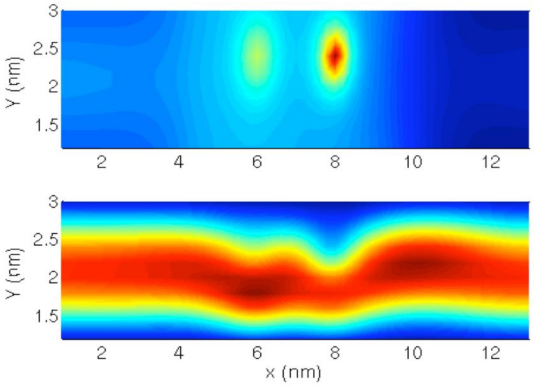

Figure 8 The potential (Upper panel) and current density (Lower panel) at the plane x=2.0 nm for the device of Fig. 7

Fig.7 shows the distribution of the potential and the x component of the current J_x in the x=2.0 (y,z) plane. The repulsive potential of the two impurities squeezes the meandering current in all three directions resulting in places in a current flow almost perpendicular to the channel.

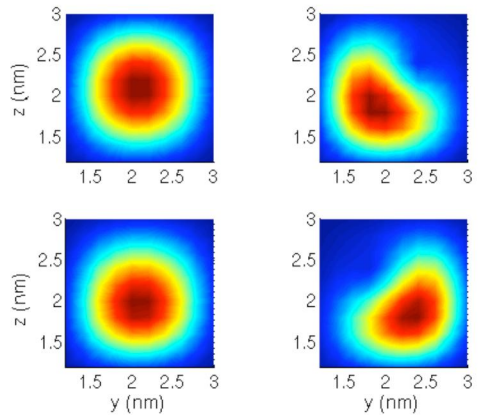

Figure 9 The electron density at different cross sections along the channel: Upper left at x=2 nm, Upper right at x=6 nm, Lower left at x=7nm and Lower right at x=8nm

Fig. 8 shows the distribution of the potential and the x component of the current J_x in the y=2.0nm (x,z) plane which is orthogonal to the plane from Fig. 7. In this plane one of the impurities is off the plane allowing the current to flow more in alignment to the channel. However a three dimensional current flow can still be observed around the other impurity center (x,z) plane.

The electron density in different cross sections along the channel is shown in Fig. 9. The cross sections are chosen in order to illustrate the effect of the repulsive potential on the wave function shape. The symmetry of the wave function in the square cross section is totally distorted clearly illustrating the non-perturbative nature of the impurity potential.

IV. Conclusions

We have shown that our recently developed full 3D NEGF solver can handle the highly inhomogeneous potentials associated with stray dopants, which result in substantial changes in current and electron densities in the device cross sections. The current meanders in a completely 3D pattern, which cannot be described by the 1D mode-space approach. In the cross section the symmetry of the wave function can be totally distorted, as we observed in the case of the two impurities in the channel.

The data supports the hypothesis that 3D flows are less sensitive to discrete impurities than corresponding 2D flows. The fact that the current has more freedom to flow around the impurity in 3D geometries, as compared to 2D geometries where the impurities are treated as line of charges (cylindrical symmetry) implies that the potential of the impurities are obviously overestimated in 2D

References

[1] M.V. Fischetti ,S. E. Laux and A. Kumar, "Simulation of quantum electronic transport in small devices: A master equation approach" IEDM Tech. Dig. pp. 467, 2003

[2] B. A. Biegel and J. D. Plummer, "Comparision of self-consistency iteration options for Wigner function method of quantum device simulation." Phys. Rev. B 54, pp. 8070, 1996

[3] A. Svizhenko, M. P. Anantrqam, T. R. Govindan, and B. Biegel, "Two-dimensional quantum mechanical modeling of nanotransistors." J. App. Phys. 91, pp. 2343, 2002

[4] J. Wang and M Lundstrom, "Does source-to-drain tunneling limit the ultimate scalling of MOSFETs?" IEDM Tech. Dig. pp. 707 2002

[5] M. Bescond et al., Proc. ESSDERC'05, pp. 221 2005

[6] R. Venugopal, Z. Ren, S. Datta and M. Lundstrom, "Simulating quantum transport in nanoscale transistors: Real versus mode-space approaches" J. App. Phys. **92**, pp. 3730-3739 2002