NESS: new flexible Nano-Electronic Simulation Software

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***Abstract*— In this paper, we present an integrated simulation environment called NESS that enables the modelling of nano CMOS transistors with different models and degrees of complexity. Thanks to its unified simulation domain for all solvers, NESS offers the possibility to consider confinement-aware band structures, generate different sources of variability and assess their impact on the figures of merit using different transport models. NESS is also a modular open-ended simulation environment that can be easily extended to include new modules such as nano-interconnects and a direct Boltzmann solver.**

Keywords—NEGF, Kubo-Greenwood, Drift-Diffusion, Tight-Binding, Effective Mass, Integrated Simulation Environment, Variability.

I. Introduction

With 7nm CMOS technology generation in prototyping, the semiconductor industry has entered the true nanotechnology era when characteristic transistor dimensions are measured in nanometres instead of tens of nanometres. Quantum confinement and quantum transport phenomena dominate the transistor characteristics and have to be taken into account in simulations together with the charge and matter granularity and the complexity of the interface transitions. Simulation tools with different level of complexity including drift-diffusion (DD) with quantum corrections [1], 3D ensemble Monte Carlo (MC) [2], MultiSubband (MS) 2D [3] and 1D MC [4], direct Boltzmann Equation solvers [5], Non-Equilibrium Green's Function (NEGF) simulators in ballistic regime [6] and with scattering [7] have been developed by different software vendors and research groups. However, these simulators usually work in isolation and it is difficult to carry out consistent simulations for a particular transistor structure highlighting and understanding the areas of applicability and the additionality of simulation techniques with increasing complexity listed above. In this paper, we present a flexible and open-ended simulation environment developed in Device Modelling Group at The University of Glasgow that enables simulations, with increasing complexity and physical content, to be carried out in a single nano-transistor represented by unified simulation domain.

II. Overview

Fig. 1 shows the modular structure of our simulation environment called NESS (Nano-Electronic Simulation Software). It contains five main modules: Input Language (IL), Material Database (MD), Structure Generator (SG), Solvers, and Outputs. The IL is written in Python, allowing users to specify the input instructions for the SG and the solvers to be used in transistor simulations. MD provides the relevant material parameters for each solver. The SG allows the creation and the configuration of the 3D device structures, doping profiles and the generation of variability sources such as random discrete dopant (RDD), line edge roughness (LER), and metal gate granularity (MGG). Examples of SG capabilities are illustrated in Fig. 2.

The transport and confinement effective masses and nonparabolicy to be used in transport models can be extracted from atomistic simulations such as Density Functional Theory

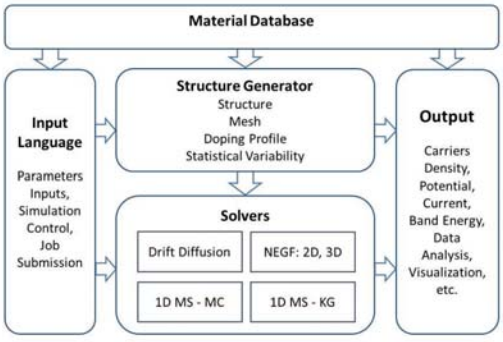

Fig. 1. The modular structure of NESS.

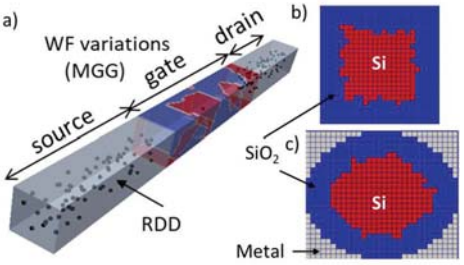

Fig. 2. a) Schematic view of nanowire FETs with RDD and MGG. Nanowires with LER having b) square and c) elliptic cross-sections.

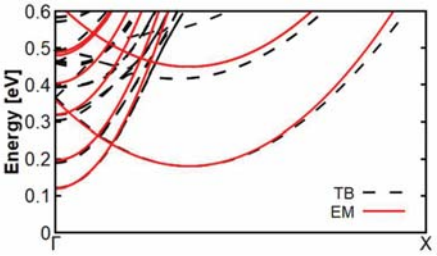

Fig. 3. The conduction band structure of 4×4 nm^2 Si nanowire from tight-binding and effective mass Hamiltonians. The conduction band edge of bulk Si is set to 0.0 eV.

and/or empirical Tight-Binding (TB) method. An example of effective mass extraction for a [100]-oriented 4×4 nm^2 square Si nanowire using $sp^3d^5s^*$ TB method [8] is shown in Fig. 3. This figure shows that the band structure obtained from the effective mass (EM) Hamiltonian with the calibrated effective masses is in good agreement with the one obtained with the TB Hamiltonian, especially at low energies which are the most relevant for transport calculations. Herein, the first and second subband energies are taken into account to calculate the confinement effective masses. All pre-caclualted effective masses are stored in the MD.

III. Transport Models

A. Drift diffusion

This classical DD solver is based on the Sharfetter-Gummel discretisation of the semiconductor equation using Bernoulli functions. Fig. 4 shows the drain current *vs* gate voltage characteristics (I_D-V_G) obtained by this solver for a square NWFET. Different mobility degradation models have been implemented to capture the effects of doping (Masetti model [9]), and vertical and longitudinal electric fields (Yamaguchi [10] and Caughey-Thomas [11] models respectively). As expected, the drain current reduces when switching on these models. Quantum corrections are being included based on 2D-Poisson-Schrödinger (PS) solutions in each cross-sectional discretization plane. The DD potential profile and charge density are used as initial guesses for the NEGF and 1D MS-MC solvers.

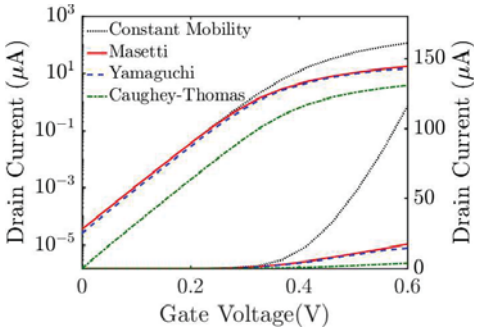

Fig. 4. I_D-V_G characteristics at V_{DS} = 0.6 V for a 4x4 nm^2 square NWFET using different mobility models in the DD solver.

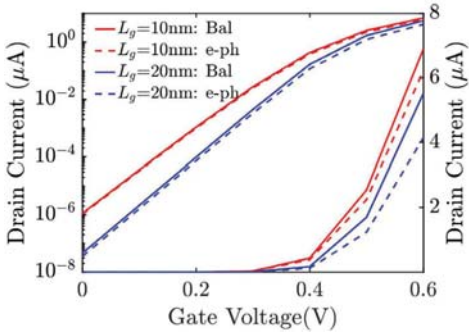

Fig. 5. NEGF I_D-V_G characteristics at V_{DS} = 0.6 V for a 4x4 nm^2 square NWFET. Solid lines are for ballistic simulations and dashed ones are for simulations including acoustic phonons.

B. Non-Equilibrium Green's Function

This formalism allows a quantum treatment of charge transport to capture quantum phenomena in nano-devices such as tunnelling, coherence and particle-particle interactions. The electrons are described in this module by EM Hamiltonian. By solving self-consistently Poisson and NEGF transport equations in coupled mode-space, we obtain the charge density, the potential profile and the current in the device. We can either consider the electron-phonon interactions or neglect them to study the transport in the ballistic limit and assess the impact of phonons on device operation [12]. An example of such a study is presented in Fig. 5, where we plot the I_D-V_G characteristics of a 4x4 nm^2 cross-section NWFET with two different gate lengths. The transverse and longitudinal effective masses are extracted from the nanowire full-band structure shown in Fig. 3. Our simulation tool captures the increase in ballisticity and subthreshold slope along with the decrease of the threshold voltage (V_{th}) when the gate length is reduced form 20 nm to 10 nm [7]. The ballisticity is defined as the ratio of the current including phonon scattering to the ballistic one. It is also possible to investigate the impact of LER, RDD and MGG on quantum transport (Fig. 6) and perform statistical simulations to study the variability of the most important figures of merit of a device (Fig. 7). We generate RDD and LER using the same technics described in ref. [13].

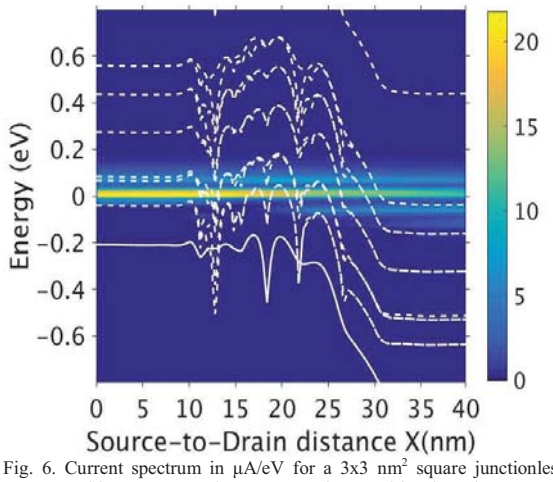

Fig. 6. Current spectrum in μA/eV for a 3x3 nm^2 square junctionless NWFET with L_G = 10 nm in ON-state. The Fermi levels at the source is the energy reference (0eV) and V_{DS} = 0.6V. The subbands are plotted in dashed lines. The solid line is the bulk conduction band in the middle of the device. Average doping density in the device is $N_D = 10^{20}$ cm^{-3}.

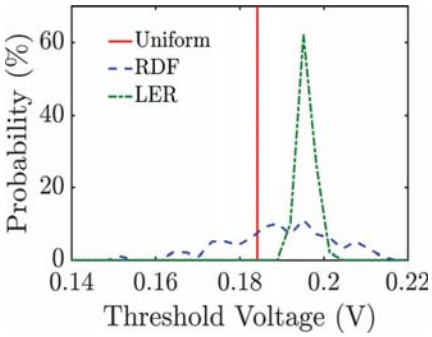

Fig. 7. Threshold voltage variability due to RDD and LER in 3x3 nm^2 square Si Nanowire, with L_G = 9 nm and N_D = 10^{20} cm^{-3}. Root mean square fluctuation for LER is 0.2 nm, and the correlation length is 1nm.

Fig. 7 shows comparison of the threshold voltage variability associated with RDD and LER. Square NWFETs with a 3x3 nm^2 cross-section are used for this analysis, and the root mean square fluctuation and the correlation length for LER are assumed to be 0.2 and 1 nm, respectively. The reference data (solid line) is obtained without variability sources. As we can see in this figure, the variability induced by RDD is more important than the one induced by LER for NWFETs with very small cross-sections.

It is also important to highlight the relevance of electron-phonon interactions even for short gate lengths when considering a variability source such as RDD [13]. Indeed, optical phonons broaden the impurity states. As shown in Fig. 6, the carriers emitted from the source with a certain energy can either couple to higher energy impurity states – via optical phonon absorption – or relax to lower energies by emitting optical phonons.

Moreover, NESS allows the calculation of the band-to-band tunnelling (BTBT) in nanodevices. The BTBT is computed

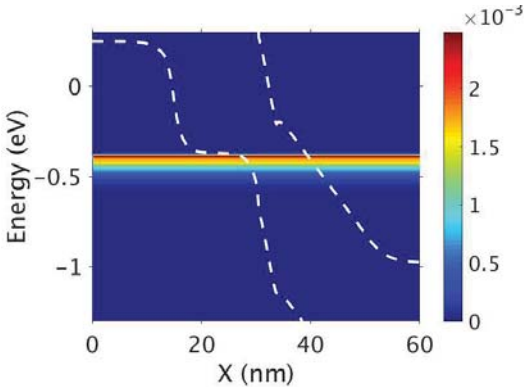

Fig. 8. Simulated ON-state current-spectra of a Si-InAs nanowire TFET. Two dopants are randomly distributed in the InAs region (x > 30 nm), corresponding to a n-type doping concentration of $N_D = 10^{19}$ cm^{-3}. The nanowire diameter is 3.5 nm. The Si region (x < 15 nm) is p-doped with N_A = 2 x 10^{20} cm^{-3}. V_{DS} = -1.0 V and the EOT = 0.46 nm. The white lines

following the approach proposed in [14]. We have implemented and adapted the Flietner [15] model to calculate the BTBT current in nanowire TFETs within the NEGF formalism, as shown in Fig. 8.

C. Kubo-Greenwood

The low-field electron mobility is one of the parameters which determines the NWFETs performance. Its main goal is to identify the scattering mechanism that limits the mobility, which is of special interest when optimizing a technology. A 1D multisubband Kubo-Greenwood (KG) simulator [5] has been integrated in order to calculate the low-field electron mobility. The approach herein considered is based on the long-channel simulation model, in which multiple cross sections of the device are simulated applying a low and constant electric field in the transport direction. The required potential distribution and the corresponding eigenfunctions are pre-calculated using the NEGF module. These quantities are included in the scattering rates and then the mobilities associated with each mechanism are calculated applying the Kubo-Greenwood formula within the relaxation time approximation. Acoustic and optical phonons, surface roughness, ionized impurity and alloy scattering rates are integrated accounting for the multisubband effects. Finally, the total mobility is estimated as a function of the individual ones by means of Mathiessen rule. The advantage of this combined semi-classical strategy in comparison with purely quantum transport is that it allows a fast computation of each mechanism separately and then combining them using Mathiessen rule. In particular, it is of special interest for devices with large cross sections, whereas the error induced by the Mathiessen rule in thinner devices can be compared to MS-MC and NEGF modules integrated in NESS.

Fig. 9 shows the total mobility, which includes both phonon and surface roughness scattering mechanisms, as a function of the sheet density for square and circular NW structures when their widths are 3nm, 5nm, and 8nm, respectively. Let us highlight two different results illustrated in Fig. 9. On one side, both the cross section shape and width modify the total mobility

due to the overlap factor dependence on the NWFET area. On

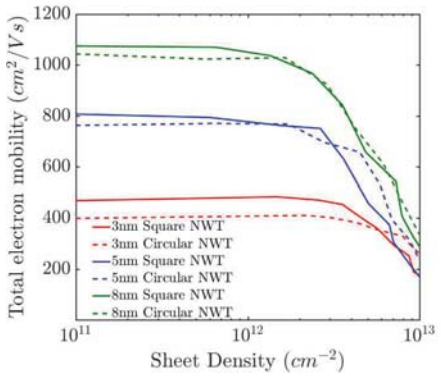

Fig. 9. Total mobility, which includes both phonon and surface roughness scattering mechanisms, as a function of the sheet density for square and circular NWT shapes and 3nm, 5nm, and 8nm widths.

the other side, the surface roughness scattering is more pronounced at higher sheet density, and becomes the dominant mechanism at lower sheet density when the NWFET width increases.

D. 1D MS-MC

This module, which is currently under development, solves the 1D Boltzmann equation through the Monte Carlo method accounting for multi-subband effects and independent quantum transport modules.

IV. Conclusion

We have presented the concepts and the current stage of development of a new flexible nanotransistor simulator NESS. It is an open-ended simulation tool offering a unified simulation domain for different solvers and allowing the study of device figures of merit using models with different degrees of complexity. We demonstrate in this paper the possibility for the user to import confinement-aware band structures, generate variability sources and assess their impact using Drift Diffusion, NEGF or Kubo-Greenwood solvers. The modular architecture of NESS allows easy addition of new simulation modules which in future may include nano-interconnects and direct Boltzmann equation solvers.

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