Enhanced Capabilities of the Nano-Electronic Simulation Software (NESS)

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***Abstract*—The aim of this paper is to present a flexible TCAD platform called Nano-Electronic Simulation Software (NESS) which enables the modelling of contemporary future electronic devices combining different simulation paradigms (with different degrees of complexity) in a unified simulation domain. NESS considers confinement-aware band structures, generates the main sources of variability, and can study their impact using different transport models. In particular, this work focuses on the new modules implemented: Kubo-Greenwood solver, Kinetic Monte Carlo solver, Gate Leakage calculation, and a full-band quantum transport solver in the presence of hole-phonon interactions using a mode-space $k \cdot p$ approach in combination with the existing NEGF module.**

***Index Terms*—Integrated Simulation Environment, Drift-Diffusion, Kubo-Greenwood, Gate Leakage, Kinetic Monte Carlo, Non-Equilibrium Green's Function, Six band k.p, Effective mass, Variability**

I. Introduction

As the 5 nm CMOS technology is being prototyped, the need for advanced nano-transistor transport simulation has increased. In particular, new device architectures and concepts rapidly evolve and add new simulation requirements. Since the quantum confinement and quantum transport phenomena are dominating the nano-scale transistor characteristics, they have to be incorporated in simulations. Moreover, the inclusion of statistical variability sources (such as charge and matter granularity and the complexity of the interface transitions) when the transistor dimensions are in the nanometer range are mandatory. Over the years, simulation tools with different levels of complexity and related computational cost have been developed by different software vendors and research groups, generally working in isolation: from classical (e.g. Drift-Diffusion (DD) [1]); through semi-classical (e.g. Monte Carlo (MC) [2] or direct Boltzmann Transport Equation (BTE) [3] solvers); to quantum transport solvers (e.g. Non-Equilibrium Green's Function (NEGF) [4]). In this work, we outline the development advances of the Nano-Electronic Simulation Software (NESS) [5] developed in the Device Modelling group at University of Glasgow, which is a flexible and modular platform combining different simulation paradigms in a unified simulation domain. Accordingly, it enables consistent simulations with techniques of varying complexity for a particular transistor structure highlighting and understanding the areas of applicability.

This project has received funding from EPSRC UKRI Innovation Fellowship scheme under grant agreement No. EP/S001131/1 (QSEE), No. EP/P009972/1 (QUANTDEVMOD) and No. EP/S000259/1(Variability PDK for design based research on FPGA/neuro computing); and from H2020-FETOPEN-2019 scheme under grant agreement No.862539-Electromed-FET OPEN.

II. Overview of NESS

Fig. 1 shows the five main modules of our simulation environment NESS: structure generator, effective mass extractor, material database, solvers, and outputs. First, the structure generator allows the creation and configuration of the 3D device structures [6], [7], including the following main variability sources: random discrete dopant (RDD), line edge roughness (LER), and metal gate granularity (MGG). Second, the effective mass extractor [8] can calculate the correct electron effective masses, in both confinement and transport directions, from the first principle simulations of the electronic bandstructure of nanowire transistors (NWTs) with technologically relevant cross-sectional area, shape, and transport orientations. Third, the material database provides the relevant material parameters for each solver, such as the work-function, affinity, or scattering parameters. Furthermore, the effective masses can be provided for each material from

density functional theory (DFT), tight-binding (TB) methods, or directly from our effective mass extractor.

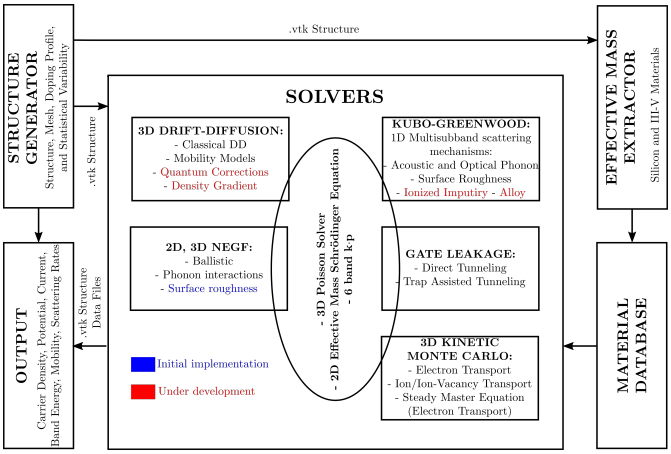

Fig. 1: Flowchart of NESS detailing its modular structure.

Fourth, different transport simulation solvers, with increasing computational complexity and cost, have been already implemented [5]. In general, each of them is self-consistently solved with the 3D Poisson and the 2D Schrödinger equations. The classical DD solver is based on the Sharfetter-Gummel discretisation of the semiconductor equation using Bernoulli functions. It contains different mobility models as well as quantum corrections based on Poisson-Schrödinger solutions [9], and density gradient. The coupled mode-space NEGF solver allows a quantum treatment of charge transport in nanodevices, naturally capturing quantum transport phenomena, such as tunnelling, coherence and particle-particle interactions. This solver can consider phonon scattering in addition to the transport in the ballistic limit. Furthermore, the NEGF solver implemented in NESS allows the calculation of band-to-band tunneling (BTBT) by using the Flietner model to compute the current in heterostructures with direct band gap [10] and the study of surface roughness (SR) scattering mechanism [11]. Finally, the simulation results are stored in text files (i.e. current, charge concentration) and also in vtk format for easy visualisation with freeware software, such as ParaView.

Fig. 2 shows the I_D vs. V_{GS} characteristics for n-type square 3nm Si NWTs with L_G=20nm considering both the classical DD module as well as the NEGF module assuming ballistic and dissipative transport with: *(i)* acoustic phonon (Ac), *(ii)* g-type optical phonon (Op); and *(iii)* SR scattering mechanisms. The new modules in NESS are described in detail in the following section.

III. New Modules in NESS

A. Kubo-Greenwood mobility module:

A 1D multisubband Kubo-Greenwood (KG) simulator [12] has been integrated in NESS in order to calculate the low-field electron mobility. This semi-classical approach combines the quantum effects based on the 1D multi-subband scattering rates of the most relevant scattering mechanisms in NWTs and

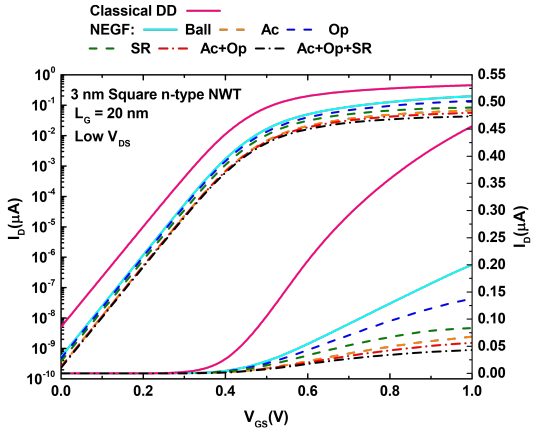

Fig. 2: I_D vs. V_{GS} characteristics for n-type square 3nm Si NWTs with L_G=20nm using the classical DD and the NEGF modules, assuming ballistic and dissipative transport with acoustic (Ac), g-type optical (Op) phonon and surface roughness (SR) scattering mechanisms

the semi-classical BTE by applying the KG formula within the relaxation time approximation. In Fig. 3, we present a comparison of the KG mobility with the mobility computed by the NEGF module considering the same scattering mechanisms as in Fig. 2: Ac, g-type Op (which corresponds to intravalley transitions) and SR. Apart from the scattering mechanisms included in Fig. 3, the f-type Op phonon (intervalley transitions) and the ionized impurity are also implemented in NESS.

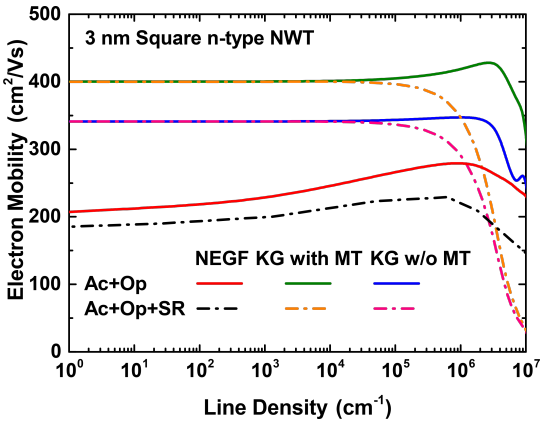

Fig. 3: Comparison of the electron mobility for a square 3nm Si NWT computed using NEGF and KG solvers combining acoustic (Ac) and g-type optical (Op) phonon scattering, and all the mechanisms (Ac + Op + surface roughness SR).

As this solver is based on the long-channel device approximation, the first step is to pre-calculate the required subband levels (E_l) and the corresponding wavefunctions (ξ_l) using a self-consistent Poisson-Schrödinger simulation in the presence of a low electric field in the transport direction. Currently, this pre-calculation is carried out using the NEGF module in NESS. The second step is to use these quantities to compute the scattering rates whose equations are directly derived from the Fermi golden rule [12]. Finally, the total mobility is estimated using either the Matthiessen rule, or

by directly summing the scattering rates of each mechanism and the total mobility for each subband based on the KG formalism. In general, the advantage of both semi-classical alternatives to compute the total mobility in comparison to purely quantum transport simulations is that the rates are individually computed and then combined, hence reducing dramatically the computational cost.

B. Kinetic Monte Carlo module:

A kinetic Monte Carlo (kMC) module has been added to NESS, which is used to model memory devices with metal-oxide layers (e.g. Flash memory, RRAM, etc.). The kMC accounts for ionic and electronic transport, ion and ion-vacancy generation and recombination. Note that the diffusion barrier of the vacancies are relatively high, therefore we neglect the ion-vacancy transport [18]. In order to model the electronic transport, a comprehensive set of physics-based models are included to capture the Poole-Frenkel emission, Direct and Fowler-Nordheim (FN) tunneling, defect to defect tunneling, elastic and inelastic electrode to defect tunneling and vice versa tunneling models [16]. The electronic transport can also be modeled using the steady state master equation as in Ref. [17]. The electronic KMC (or steady state master equation), which is coupled to the ionic KMC, is used to model the RRAM devices [18] and the different aspects of the flash memory operation. An example for ion vacancy distributions for TiN/SiOx/TiN structure, during the forming, reset (overlapping of forming and reset ion vacancies) and set (overlapping of reset and set ion vacancies) processes are depicted in Fig. 4. It is important to highlight during the reset process that there are less vacancies near the bottom terminal. Fig. 5 shows the RRAM characteristic including forming, reset and set trajectories of a SiOx based RRAM. For these simulations, the steady state master equation was used to model the electronic transport while the ion dynamics were modeled using the kMC approach.

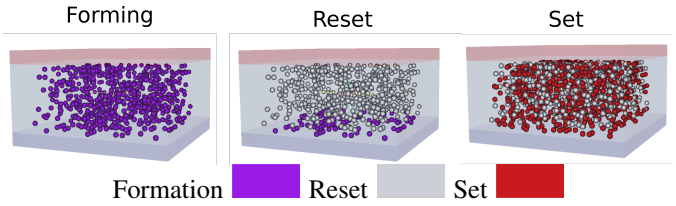

Fig. 4: Ion vacancy distributions for TiN/SiOx/TiN structure, during the forming, reset (overlapping of forming and reset ion vacancies) and set (overlapping of reset and set ion vacancies) processes.

C. Gate Leakage module:

We have implemented a module to calculate the gate leakage current in NESS. The gate leakage current is considered to be the sum of direct tunneling, FN tunneling, and trap assisted tunneling (TAT). The direct and FN tunneling are modelled using the Tsu-Esaki formulation [13], while the TAT is calculated using the methodology as proposed in Ref. [14]. This flexible module allows the user to set the

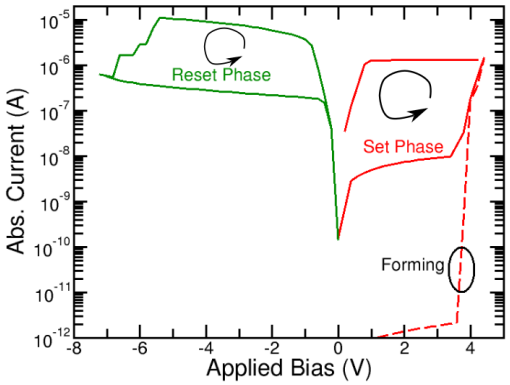

Fig. 5: Simulation characteristic of a bipolar SiOx based RRAM device. The compliance current of 1μA was enforced in the simulation.

trap parameters including trap density, energy and number of material dependent parameters. The module can also account for the impact of different sources of variability like oxide-semiconductor interface roughness, random discrete dopants, and random interface charges. Fig. 6 shows a comparison between the gate leakage calculated using the implemented module and experimental results.

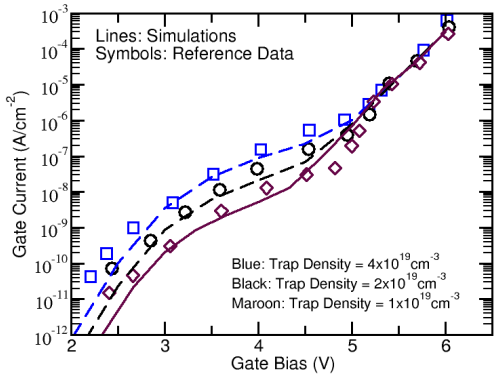

Fig. 6: Comparison between the reference gate current (symbols) and the simulated results (solid lines). The reference data is from [15].

D. Six Band $k \cdot p$ NEGF simulation capabilities:

We have implemented a mode-space full-band quantum transport solver with hole-phonon interactions by adding a six-band $k \cdot p$ Hamiltonian to the existing NEGF module in NESS [19]. The Hamiltonian is first unitary transformed from real-space to a reduced-order Hamiltonian discretized in the K-space which is constructed from sampling the Brillouin zone and obtaining the Bloch modes significant to the transport. The mode-space Hamiltonian is then generated by unitary transforming the reduced-order Hamiltonian in K-space [20], [21]. The expressions for the hole-phonon interactions self-energies within the mode-space representation are based on the self-consistent Born approximation and are given in Ref. [19]. Fig. 7 shows the efficient simulations of p-type square

3 nm Si NWT considering the most common crystallographic orientations ([100, 110, 111]) with coherent and dissipative transport. The energy transfer due to scattering in NEGF is shown in Fig. 8 where the LDOS is represented for the device considered in Fig. 7 with transport direction [100] and gate voltage of -0.6 V.

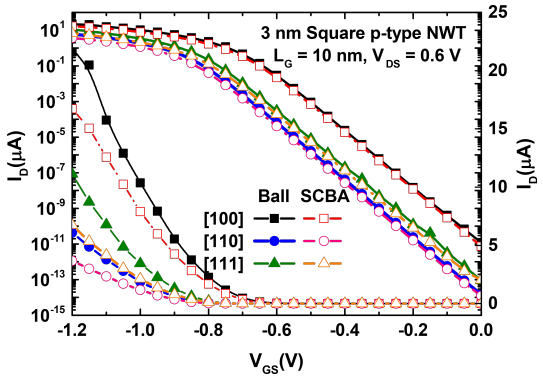

Fig. 7: I_D vs. V_{GS} characteristics for p-type square 3 nm Si NWTs considering the most common crystallographic orientations ([100, 110, 111]) with coherent and dissipative transport. The results have been simulated making use of the mode-space full-band quantum transport solver included in NESS by combining a six-band $k \cdot p$ Hamiltonian and the existing NEGF module.

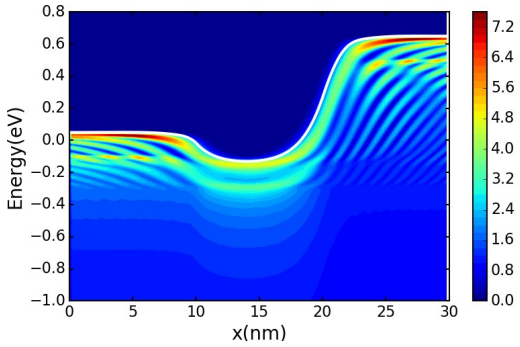

Fig. 8: LDOS for the device simulated in Fig. 7 with transport direction [100] and gate voltage -0.6 V. The white line corresponds to the conduction band.

IV. Conclusions

In this work, we have presented a general overview and the current stage of development of our flexible nanotransistor simulator NESS, with focus on the new modules implemented: Kubo-Greenwood solver, Kinetic Monte Carlo solver, Gate Leakage calculation, and a full-band quantum transport solver in presence of hole-phonon interactions using a mode-space $k \cdot p$ approach in combination with the existing NEGF module. The NESS modular architecture and unified simulation domain have allowed us to include solvers with different complexity and simulation techniques to study nanoelectronic structures in different areas of research and applications. The environment makes also easy its future expansion with new modules/solvers such as nano-interconnects and a direct Boltzmann solver.

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