Efficient Coupled-mode space based Non-Equilibrium Green's Function Approach for Modeling Quantum Transport and Variability in Vertically Stacked SiNW FETs

V. Thirunavukkarasu*[1], H. Carrillo-Nunez[1], F. D. Alema[1], S. Berrada[1], O. Badami[1], C. Medina-Bailón[1], T. Datta[1], J. Lee[1], Y. Guen[2], V. Georgiev[1] and A. Asenov[1]

[1]School of Engineering, University of Glasgow, Glasgow G12 8LT, Scotland, UK.
[2]Department of Electrical Engineering, Xian Chiao Tung University, People Republic of China.
e-mail* nanodhasan@gmail.com

Abstract— In this paper we present state of the art coupled-mode space based Non-Equilibrium Green Function approach for modeling quantum transport accurately in the vertically stacked Silicon nanowire (SiNW) FETs. Random discrete dopants (RDD) and metal grain granularity (MGG) induced variability in stacked SiNW FETs are also investigated. Furthermore, charge spectrum, current spectrum w.r.t. sub bands and the space-resolved Local Density of States (LDOS) corresponding to the location of band edge are analyzed in detail. The newly developed flexible and computationally efficient models implemented in quantum transport simulation tool NESS provides valuable insights on the effect of RDD and MGG variability on Sub-Threshold Swing (SS), Threshold Voltage (V_{TH}) shift, On/Off Current (I_{ON}/I_{OFF}) ratio and quantum confined charge transport mechanism.

I. Introduction

As CMOS technology advances, logic devices are aggressively scaled [1]. It is very crucial to develop accurate models to investigate the ultra-scaled nano devices as the quantum charge transport is highly influenced by the strong confinement effects in quantum regime [2-4]. Stacked Gate All Around (GAA) transistors promises better gate electrostatics and high performance in sub 7nm advanced technology nodes [5-7]. To investigate short channel effects, quantum charge confinement, ballistic and diffusive transport, tunneling and variability induced effects accurately advanced tools with quantum NEGF approach is a must. In this work, we demonstrated quantum simulation tool NESS *(i)* capability to handle complex device structures and sophisticated geometries; *(ii)* extract and investigate the quantum transport with electron-phonon interactions and *(iii)* use the fully 3D self-consistent couple-mode space NEGF formalism to model the impact of the process induced variation such as MGG or RDD using statistical ensembles of 100 devices. The impact of phonon scattering on the performance of staked-nanowire FETs is also investigated. Details on the simulation procedure is given below.

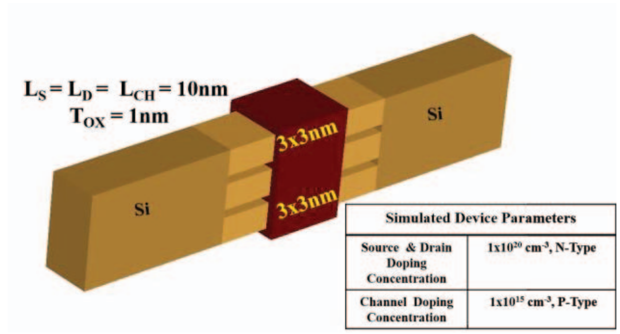

Fig. 1 Device structure of simulated Vertically Stacked Gate-All-Around Transistor with three 3 x 3nm stacked Channels. Inset shows the doping concentration used in the simulation.

II. Simulation Methodology

Assuming steady-state conditions, quantum transport is described by means of the Non-Equilibrium Green's Function (NEGF) formalism within the coupled mode-space representation [8][9], as implemented in the quantum transport simulator NESS [10] from the University of Glasgow. The NEGF solver is based on the effective-mass approximation and is self-consistently coupled with Poisson's equation. Both acoustic and optical phonon scattering are tackled within the self-consistent Born approximation (SCBA) [11]. Using the latter, the electron-phonon interactions are incorporated in the NEGF formalism through self-energies in terms of the retarded/lesser/greater-than Green's function $\Sigma^{R/</>}=M_{ep}\ G^{R/</>}$, where M_{ep} is the electron-phono coupling strength. Exact expression of the electron-phonon self-energies can be found in Refs. [12] [13]. In practice, both NEGF approach and SCBA are solved self-consistently using a recursive algorithm [11] until the criteria of convergence for both electron and current densities are reached.

We examined the quantum charge transport properties in stacked GAA transistors with three stacked GAA 3x3 channels as shown in Fig. 1 and compared the transfer characteristics of statistical simulations for 100 samples with *(i)* only RDD, *(ii)* only MGG and *(iii)* both RDD and MGG variability sources. Dopants in the source and drain regions are randomly chosen from a Poisson distribution, placing them by means of a probability rejection technique. The mean is determined by the

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doping concentration multiplied by the volume of the RDD region. Regarding MGG, the grains in the metal gate region are generated by using the Voronoi algorithm [14]. The work-function for each grain can be either 4.4 or 4.6 eV with the probability of 40% or 60% based on previous experimental results [15]. It was reported that, as the grain size increases, the more significant variability is observed, meaning that the small average grain size causes less variability [14]. Therefore, the average grain size of 3.0 nm used in this paper is small enough to expect a relatively less MGG-induced variability. The aforementioned models and an efficient NEGF recursive algorithms are implemented in NESS to the compute physical quantities like carrier density and current. Our main findings are summarized as follows.

III. RESULTS AND DISCUSSIONS

Fig. 2 compares the ballistic and scattering current at low bias V_{DS}= 0.05V with and without RDD+MGG for a 3x3 nanowire GAA device. The impact of scattering with RDD+MGG is not very significant. Hence to reduce computational cost, for 3x3 stacked nanowire statistical simulation of 100 devices ballistic simulations are considered. Fig. 3 shows the transfer characteristics (I_d-V_g) of the 100 three-channels stacked 3x3nm nanowire devices. I_d obtained is normalized by the effective width of the three stacked 3x3nm nanowires.

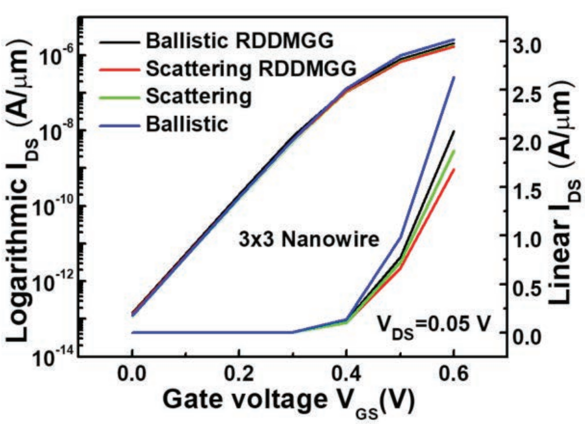

Fig. 2 Id-Vg Transfer Characteristics of 3x3 square nanowire devices in ballistic and considering phonon scattering with and without RDD+MGG. Impact of scattering is less severe in extremely-scaled NW GAA devices. Vds of 0.05V is applied.

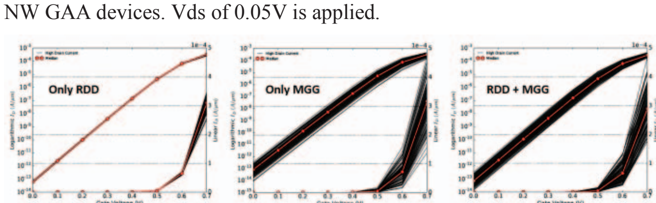

Fig. 3 Id-Vg Transfer Characteristics of statistical ensemble of 100 devices with only RDD, only MGG and both RDD+MGG. Median is highlighted as a line with red circles. Vds of 0.6V is applied.

The devices are simulated in three different setups. Devices with only RDD, only MGG and both RDD+MGG are considered. RDD has less impact on I_{on} current. Clearly the RDD is less significant compared to huge variability due to MGG which is evident from the transfer characteristics at V_{ds}=0.6V. The mean values of the drain current obtained is indicated in red.

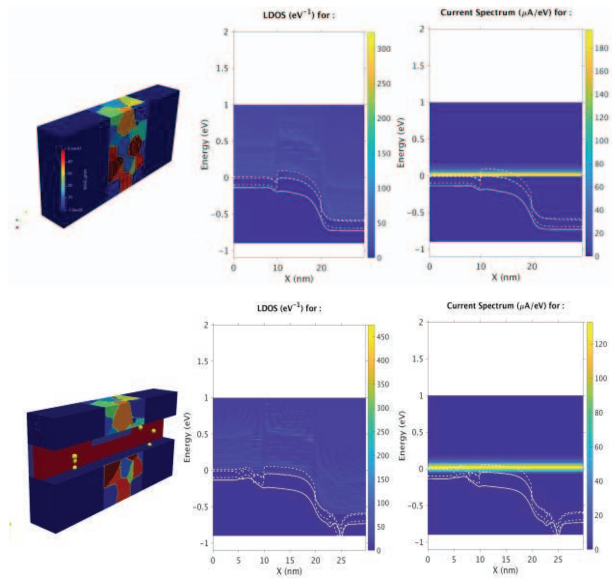

Fig. 4 Illustration of simulated Stacked Gate-All-Around Transistor with MGG and RDD+MGG along three 3 x 3nm stacked Channels. Space-resolved LDOS and Current Spectrum shows the impact of RDD and MGG on quantum-confined charge transport in sub bands.

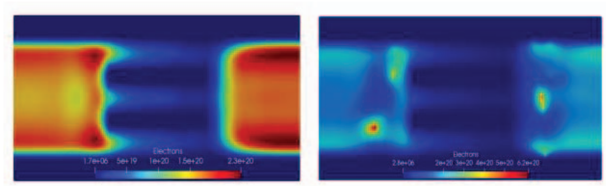

Fig. 5 Electron Density distribution in Stacked SiNW GAA without and with RDD. Random Dopants impacts the charge distribution.

Fig. 4 illustrates the MGG and RDD+MGG devices simulated. The current spectrum clearly indicates the impact of RDD in S/D region and MGG generated in the device along the transport direction. LDOS corresponding to the local band edge shows effect of potential barrier w.r.t. applied gate voltage. The space-resolved local density of state (LDOS) exhibits strong correlation between different electron densities which is shown in Fig. 5 for a device without RDD and with RDD. The impact of random dopants on the band edges can be seen. The Vth, Ion, Ioff probability distributions for the MGG, RDD and both RDD+MGG devices are shown in Fig. 6. The best-fit Gaussian function curve is indicated in the probability distribution plot. For devices with only RDD a standard deviation of 0.00136V,

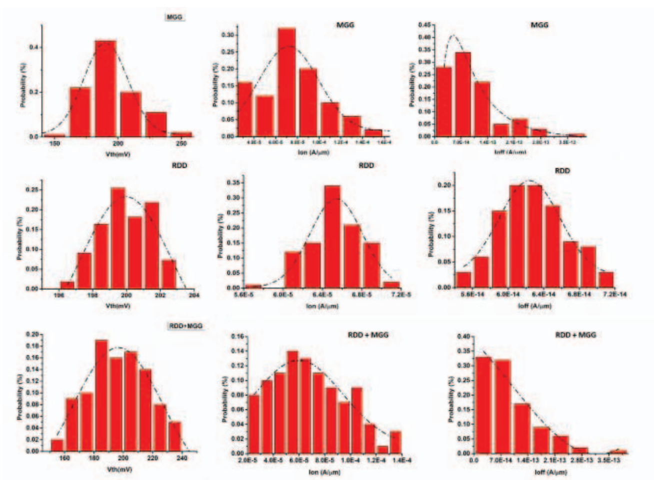

Fig. 6 Threshold Voltage (Vth), On current (Ion), Off current (Ioff) probability density distribution for three different variability samples along with best-fit Gaussian curve in black dotted-line.

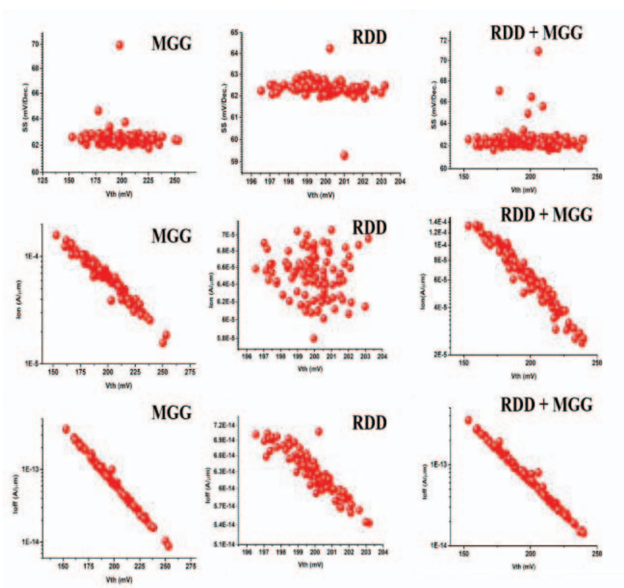

Fig. 7 Threshold Voltage (Vth) versus Subthreshold swing (SS), On current (Ion) and Off current (Ioff). RDD has significant impact on Ion. Devices with both RDD+MGG exhibit large variation in Ioff and SS.

$3.77E^{-14}$ A/µm, $2.60E^{-5}$ A/µm and 0.42mV/dec. are observed in Vth, Ioff, Ion and SS respectively. In RDD+MGG devices a standard deviation of 0.02015V, $6.78E^{-14}$ A/µm, $2.79E^{-5}$ A/µm is observed in threshold voltage (Vth), Off current (Ioff), on current (Ion) and subthreshold swing (SS) respectively. Fig. 7 shows the scatter plot of SS, Ion and Ioff variation w.r.t. threshold voltage Vth. SS can be fine-tuned by modulating the Vth further more. For RDD only devices SS_{max} of 64.5 mV/dec. and SS_{mean} of 62.36mV/dec. and for RDD+MGG devices SS_{max} of 70.94mV/dec. and SS_{mean} of 63.60mV/dec. is observed. The correlation between Vth and SS determines the performance of the stacked nanowire. Hence it is important to understand the impact metal grain granularity in stacked nanowire transistors to circumvents the performance degradation due to MGG.

IV. CONCLUSION

We examined the quantum charge transport in stacked GAA transistors and compared the transfer characteristics from RDD and MGG induced statistical variability in Stacked SiNW GAAFETs. The insights from the current spectrum and LDOS results sheds light on electron density and quantum transport which will help us to design ultra-scaled stacked GAA CMOS FETs for high performance logic devices in advanced nodes.

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