Amoroso, S., Georgiev, V., Towie, E., Riddet, C., and Asenov, A. (2014) *Metamorphosis of a nanowire: a 3-D coupled mode space NEGF study.* In: 2014 International Workshop on Computational Electronics (IWCE), 3-6 June 2014, Paris, France.

Copyright © 2014 The Authors

A copy can be downloaded for personal non-commercial research or study, without prior permission or charge

Content must not be changed in any way or reproduced in any format or medium without the formal permission of the copyright holder(s)

http://eprints.gla.ac.uk/98649/

Deposited on: 31 October 2014

Enlighten – Research publications by members of the University of Glasgow
http://eprints.gla.ac.uk

Metamorphosis of a nanowire: A 3-D coupled mode space NEGF study

Salvatore Maria Amoroso, Vihar P. Georgiev
Device Modelling Group
University of Glasgow
Oakfield Avenue, Rankine Building, G12 8LT
Salvatore.amoroso@glasgow.ac.uk

Ewan Towie, Craig Riddet, Asen Asenov
Gold Standard Simulations Ltd
Oakfield Avenue, Rankine Building
Glasgow, G12 8LT

***Abstract*— In this paper we present a 3D coupled mode space NEGF study of the quantum features of a nanoscale Gate-All-Around (GAA) silicon transistor. The bottom oxide of the structure is parameterized in order to progressively transform the nanowire in a tri-gate FinFET and the electron transport studied for several Fin widths, back-biases voltages and electron effective masses. Moreover, we address in detail the treatment of the boundary conditions at the channel interface to model the wave function penetration into the gate oxide. We report quantitative results of the charge density obtained by a simplified and a complete discretization approach.**

Keywords—Nanowire, FinFET, Quantum Transport, Schrodinger, Poisson, Non Equilibrium Green Functions.

I. INTRODUCTION

The performance gain of conventional bulk MOSFETs has become increasingly difficult through traditional scaling. Intel's shift from planar to tri-gate architectures has marked a milestone in CMOS technology history at the 22nm scaling node. Short channel effects, high leakage current, variability associated with the high channel doping, reliability associated with the high-field effects have been the main driving forces for this technological paradigm shift [1]. Nanowire transistors have been gaining increasing momentum as one of the most promising device architectures for the ultimate scaling of CMOS transistors [2]. In fact, the gate-all-around solution allows excellent channel control so that nanowires tolerate very low channel doping maintaining good electrostatic integrity, enabling the continuation of increases in performance gain until the end of the ITRS roadmap. Silicon nanowires are quasi-one-dimensional structures in which carriers are strongly confined in the 2D space perpendicular to the transport direction along which carriers exhibit their sole degree of freedom. In order to accurately study the electrical behaviour of these structures, a 2D Poisson-Schrodinger (2D-PS) solver can be coupled with a Non-Equilibrium Greens Functions (NEGFs) approach, as in [3]. *In this paper we present a detailed description of the coupled Poisson-Schrodinger-NEGF solver as employed to compute the electron charge density and charge transport in nanowire FET, considering variations in the device geometry and transport electron masses. Furthermore, we put emphasis on the treatment of the boundary conditions at the channel interface to model the wave function penetration into the gate oxide. We show how different discretization approaches to the boundary condition problem lead to different charge density profiles over all the channel cross-section.*

978-1-4799-5433-9/14/$31.00 ©2014 IEEE

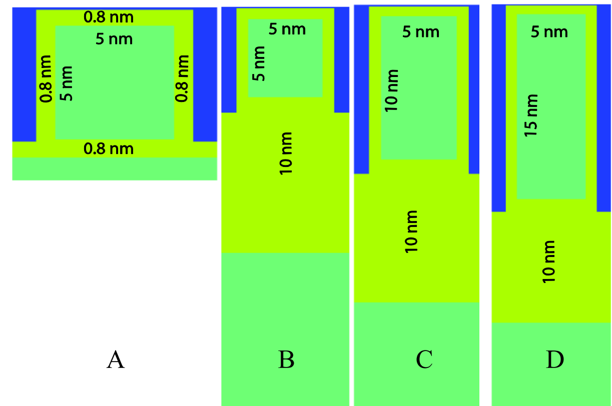

Fig. **1**. Structure of the simulated devices. Thickness of the top, left and right SiO_2 and the channel width are constant. Bottom oxide and channel height change from device A to D.

II. SIMULATION METHODOLOGY

Simulations are carried out using the quantum transport module of the GSS TCAD simulator GARAND [4]. Accurate modelling of nanoscale GAA transistors can be tackled by coupled mode space (CMS) Non-Equilibrium Green's Function (NEGF) quantum transport approach [5,6], if a sufficient number of modes is included in simulation [7]. In our work we neglect all sources of incoherent scattering, such as phonon interaction, as they have a marginal impact on our results [8]. An effective-mass Hamiltonian is used in the discretized form of the NEGF equations so that the full crystal interactions are described by the parameters $m_{eff,i}$ which are derived from tight binding calculations of silicon band structure. Please note that the tight binding approach allows us to take into account the dependence of the electron band structure on the nanowire cross-section. The CMS method splits the quantum problem into the transversal and

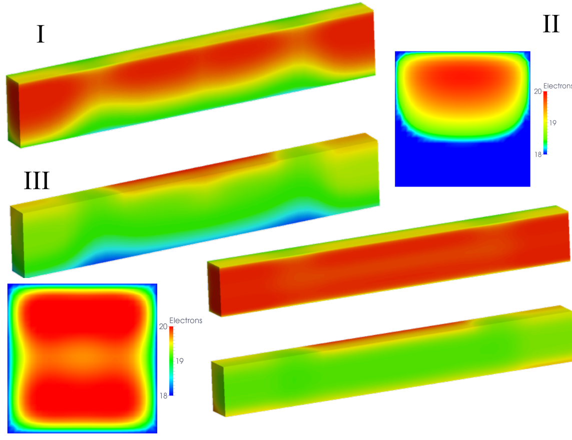

Fig. 2. Device A with bulk effective masses for Si: Electron density in a cut along the channel length (I) and on a cross-section perpendicular to the transport direction (II), and electrostatic potential (III). V_B=0V (top), V_B= 1.6V (bottom).

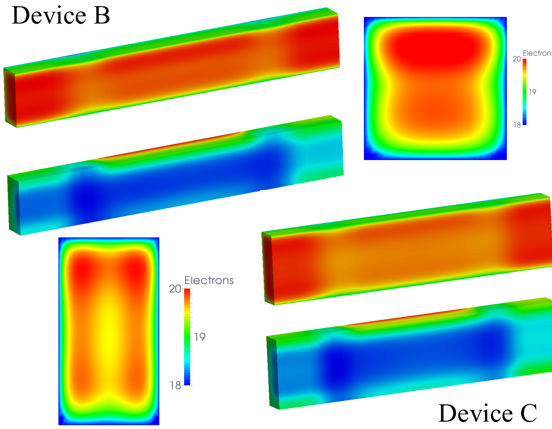

Fig. 3. The same as Fig.2, but for devices B and C.

longitudinal spaces. The transversal space provides the cross-sectional wave functions and sub-band energies by solving the 2D Schrodinger equation on each cross-section. The transport is solved in the product space of the longitudinal space with the mode space, allowing a considerable savings of computational resources with respect to a full 3D real-space approach [7]. Boundary conditions of the Green's function equations at the contacts, which are given throughout the contact self-energies, were defined by using the algorithm described in [9], while the boundary conditions at the silicon/oxide interface will be discussed in section IV. The electron density is used to calculate, self-consistently, the electrostatic potential through the Poisson's equation. The obtained solutions of the NEGF and Poisson equations are iterated in a Gummel-like loop until density and current converge [10-12].

III. IMPACT OF GEOMETRY AND ELECTRON MASSES

All calculations are performed at V_G=0.8V and V_D=50mV. Fig.1 shows a schematic view of the nanowire progressively transforming into a FinFET. In Fig.2 we report the electron density and the potential along the length section for device A, for two values of applied back bias. When V_B=0, the electron

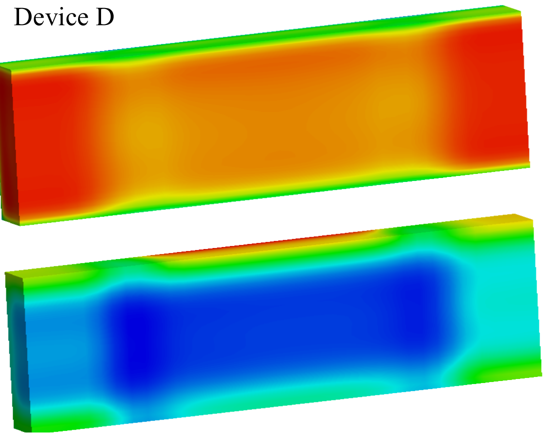

Fig. 4. Electron density (top) and potential (bottom) along the length of the channel for device D.

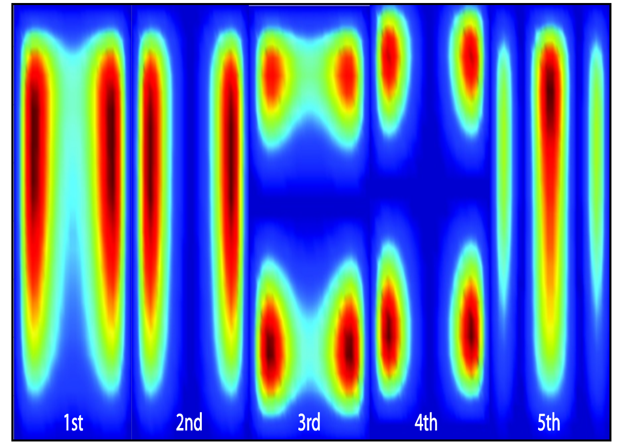

Fig. 5. Cross-section cut in the middle of the channel for device D showing the five wavefunctions with the lowest energy. The effective masses correspond to usual bulk effective masses – m_z*= 0.916m_0 and m_y*= 0.191m_0.

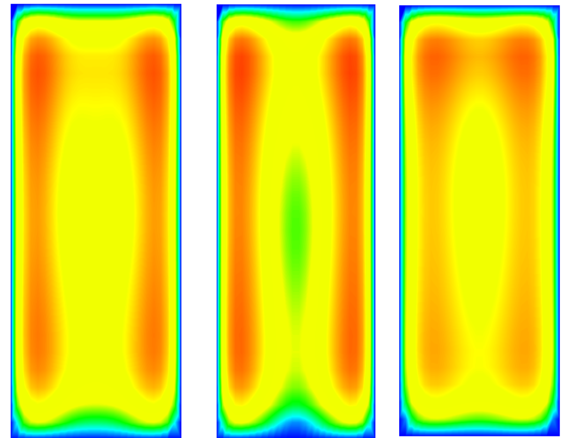

Fig.6. Electron density in the cut along the cross-section for device D: a) with bulk effective masses – m_z*= 0.916m_0 and m_y*= 0.191m_0; b) m_z*= 1.03m_0 and m_y*= 0.30m_0; c) m_z*= 2.03m_0 and m_y*= 0.10m_0.

density has a centroid close to the top interface, as the lateral gates are leveled at the same height of the Si wire, preventing a good electrostatic control of the channel bottom. More uniform charge distribution in the channel is obtained by applying a positive back-bias. In this case the structure is nearly equivalent to a GAA nanowire. In Fig. 3 – Fig.4 we show results for the devices B-D featuring different bottom oxide thickness and/or channel height. In Fig.5 we offer an insight of the first five wave-functions (squared) with lowest eigenvalues for device D. The electron density of these tri-gate structures is more uniform along the channel height than the one observed in Fig.2a because the lateral gates in devices B-D penetrate deeper in the bottom oxide allowing the electric field streamlines to better embrace the channel. Moreover, increasing the ratio between channel height and channel width, the channel is majorly controlled by the lateral gates so that the inversion layer is dominant at the Fin sidewalls (see cross-section perpendicular to transport direction in each devices). However, Fig. 6 shows that this electron distribution can significantly be modified adopting different electron effective masses in our simulation. Increasing the ratio between m_z and m_y, the charge density redistribute from the Fin sidewalls to the Fin top, offering a results similar to the ones obtained from conventional TCAD simulations [13].

IV. Impact of Wave Penetration into Gate Oxide

In this section we address the problem of wave penetration into the gate oxide. A Silicon nanowire transistor featuring a $2x2nm^2$ cross-section, a 0.8nm gate oxide and a 6nm channel length is used as template structures. We compare two discretization approaches: the first is where the wave function vanishes at the first mesh point into the oxide and the second is where the wave-function penetrates into the whole oxide. Fig. 7 presents the corresponding wave-functions for both cases, considering isotropic electron masses in the silicon (m_z=m_y=$0.33m_e$). Please note how the wave peaks in the silicon body and the wave derivatives at the interface are lowered when the eigenvectors are allowed to fully penetrate into the oxide. Moreover, we investigate the effect of anisotropic effective masses on the wave-function and density distribution. The results are presented in Fig. 8 for m_z=$0.919m_e$ and m_y=$0.19m_e$. Please note the change in eigenvectors shape due to the breaking of symmetry with respect to the case reported in Fig.7. Fig. 9 shows 1D cuts of the electron density along the y direction for isotropic masses. It is evident that the simulations with full wave penetration give rise to higher (lower) charge density at the channel interface (centre) with respect to the simulations in which the waves vanish at the first oxide mesh node.

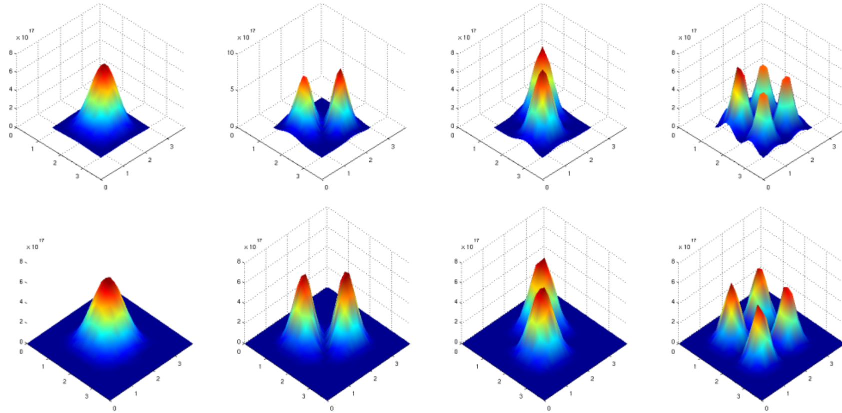

Fig.7 First four wave-functions of the nanowire. The top row is the case where the wave function vanishes at the first mesh node inside the oxide. The bottom row is the scenario with wave function penetration into the whole oxide. In this case *isotropic* effective masses for Si = $0.33m_e$ and SiO_2=$0.22m_e$ have been used.

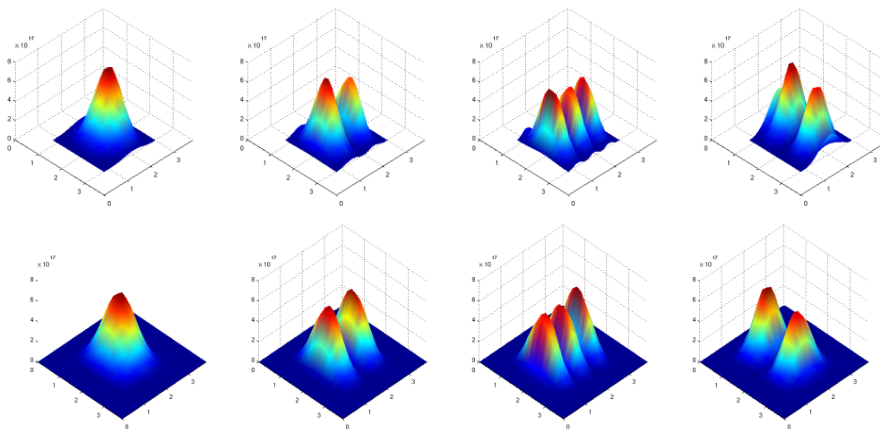

Fig.8 First four wave-functions of the nanowire. The top row is the case where the wave function vanishes at the first mesh node inside the oxide. The bottom row is the scenario with wave function penetration into the whole oxide. In this case *anisotropic* effective masses for Si – m_z=$0.919m_e$ and m_y=$0.19m_e$ have been used. The SiO_2 has effective mass equal to $0.22m_e$.

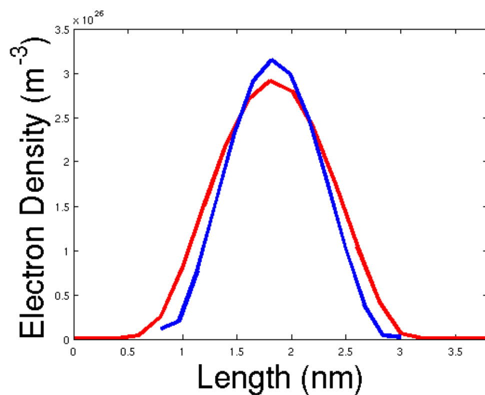

Fig. 9 1D electron density plot along the y-direction of the nanowire in the case of *isotropic* effective masses for the Si.

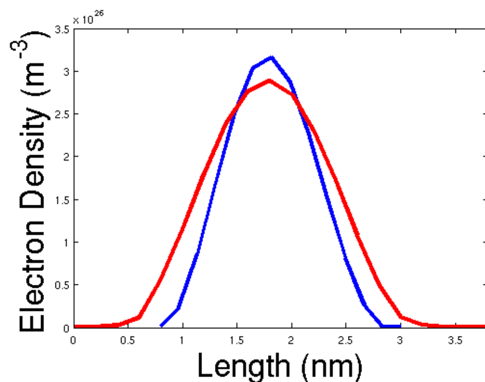

Fig. 10 1D electron density plot along the y-direction of the nanowire in the case with *anisotropic* effective masses for the Si.

Introducing anisotropic masses, exacerbate these differences in the charge density, as shown in Fig.10. From differentiating the charge density with respect the applied gate voltage it is possible to derive Capacitance-Voltage (CV) characteristics and, for example, the shift on these due to charge trapping at the channel interface. In such a way the impact of the different boundary conditions can be studied on practical problems such the oxide reliability evaluation in nanowire transistors. These applications will be reported in future publications.

V. Conclusion

We have reported a thorough 3-D simulation study of quantum transport in multi-gate nanoscale devices showing how the electron wave features change in response to geometry, effective masses and applied back-biases variations. We have also addressed how different boundary conditions in the Schrodinger-Poisson problem lead to important changes in the charge distribution in the nanowire channel.

Acknowledgment

The authors would like to thank the support given by European Commission through the FP7 grant agreement 261868 MORDRED.

References

[1] A. Asenov, B. Cheng, X. Wang, A. Brown, D. Reid, C. Millar, C. Alexander, *Simulation based transistor-SRAM co-design in the presence of statistical variability and reliability*, in IEEE IEDM Tech. Dig., 818–821, 2013.

[2] N. Singh, F. Y. Lim, W. W. Fang, S. C. Rustagi, L. K. Bera, A. Agarwal, and C. H. Tung, *Ultra-narrow silicon nanowire gate-all-around CMOS devices: Impact of diameter, channel-orientation and low temperature on device performance*, in IEEE IEDM Tech. Dig., 2006, pp. 547–550.

[3] A. Martinez, M. Aldegunde, N. Seoane, A. Brown, J. R. Barker, A. Asenov, *Quantum-Transport Study on the Impact of Channel Length and Cross Sections on Variability Induced by Random Discrete Dopants in Narrow Gate-All-Around Silicon Nanowire Transistors*,, IEEE Trans. on Electron Devices, **58**, 8, 2209-2216, 2011.

[4] www.goldstandardsimulations.com

[5] J. Wang, E. Polizzi, M. Lundstrom, *A Three-Dimensional Quantum Simulation of Silicon Nanowire Transistors with the Effective Mass Approximation,* J. Appl. Phys. **96**, 2192, 2004.

[6] G. Fiori, G. Iannaccone, G. Klimeck, *Coupled Mode Space Approach for the Simulation of Realistic Carbon Nanotube Field-Effect Transistors*, IEEE Trans. on NanoTechnology **6**, 475-480, 2007.

[7] A. Martinez, A. Brown, N. Seoane, A. Asenov., *A Comparison between a Fully-3D Real-Space Versus Coupled Mode-Space NEGF in the Study of Variability in Gate-All-Around Si Nanowire MOSFET*, Proc. of SISPAD 2009.

[8] V. P. Georgiev, E. Towie, A. Asenov, *Impact of Precisely Positioned Dopants on the Performance of an Ultimate Silicon Nanowire Transistor: A Full Three-Dimensional NEGF Simulation Study*, IEEE Trans. on Electon Devices **60**, 965-971, 2013.

[9] A. Martinez, N. Seoane, A. Brown, J. Barker, A. Asenov, *Variability in Si nanowire MOSFETs due to combined effect of interface roughness and random dopants: A full 3D NEGF study*, IEEE Trans. on Electron Devices **57**, 1626-1635, 2010.

[10] E. B. Ramayya, I. Knezevic, *Self-consistent Poisson-Schrödinger-Monte Carlo solver: electron mobility in silicon nanowires*, J. Comput. Electronics, **9**, 206-210, 2010.

[11] J. Wang, E. Polizzi, A. Ghosh, S. Datta, M. Lundstrom, *Theoretical investigation of surface roughness scattering in silicon nanowire transistors,* Appl. Phys. Lett., **87**, 043101, 2005.

[12] J. H. Luscombe, A. M. Bouchard and M. Luban, *Electron confnement in quantum nanostructures: Self-consistent Poisson-Schrodinger theory,* Phys. Rev. B, **46**, 16, 10262, 1992.

[13] L. Gerrer, S. M. Amoroso, S. Markov, F. Adamu-Lema, A. Asenov, *3-D Statistical Simulation Comparison of Oxide Reliability of Planar MOSFETs and FinFET*, IEEE Trans. on Electron Devices **60**, 4008-4013, 2013.