Solid-State Electronics 199 (2023) 108489

Contents lists available at ScienceDirect

Solid State Electronics

journal homepage: www.elsevier.com/locate/sse

Hierarchical simulation of nanosheet field effect transistor: NESS flow ☆

Daniel Nagy [a,b,*], Ali Rezaei [a], Nikolas Xeni [a], Tapas Dutta [a], Fikru Adamu-Lema [a,b], Ismail Topaloglu [a], Vihar P. Georgiev [a], Asen Asenov [a,b]

[a] *Device Modelling Group, School of Engineering, University of Glasgow, Glasgow, Scotland, UK*
[b] *Semiwise Ltd., Rankine Building, Glasgow, Scotland, UK*

ARTICLE INFO

Keywords:
Nanosheet
TCAD
Silicon
NEGF
DD

ABSTRACT

Nanosheet gate-all-around transistor devices have been an important contenders for future technology nodes. Compared to FinFETs they have superior electrostatic control. The nanosheet architecture can also be vertically stacked thus achieving higher drive current on a same footprint area compared to a single nanowire or nanosheet. Accurate device simulations are crucial for the development and the optimization of the nanosheet transistors. With this in mind, we have developed and report a hierarchical simulations flow implemented in the Glasgow Nano-Electronic Simulation Software (NESS) in order to enable the accurate simulation and optimization of the nanosheet transistors. In this work we have carried out device simulations and showed that the more accurate NEGF simulations can be used for the calibration of the classical DD simulations within one single toolbox. Additionally we showed that the EME module can be used to extract the effective masses for confined structure like the nanosheet.

1. Introduction

Nanosheet gate-all-around transistor devices have been adopted by Samsung in their 3 nm CMOS offering [1]. Compared to FinFETs they have superior electrostatic control [2,3]. The nanosheet architecture can also be vertically stacked thus achieving higher drive current on a same footprint area compared to a single nanowire or nanosheet. Accurate device simulations are crucial for the development and the optimization of the nanosheet transistors. With this in mind, we have developed and report a hierarchical simulations flow implemented in the Glasgow Nano-Electronic Simulation Software (NESS) in order to enable the accurate simulation and optimization of the nanosheet transistors [4,5].

2. Method

In Fig. 1 we have shown the modular structure of NESS. The capability of NESS in simulating novel devices has been demonstrated earlier, e.g. [6–10]. The focus in the current abstract is the flow of the essential modules for the accurate simulation of the nanosheet transistors. The relevant NESS modules include the structure generator (SG), Effective Mass Extractor (EME), Non-Equilibrium Green's Function (NEGF) and Drift–Diffusion (DD) module. All transport solvers work in a unified solution domain created by SG and are linked to a common Poisson Solver as shown in Fig. 1. In this section we briefly describe each module in the contest of the nanosheet transistors simulation.

The SG is capable of generating various structures (simulation domains) and has flexibility for the different corresponding types of devices. The generated data is stored as binary or ASCII, defining the datasets in a rectilinear grid following the topology of the coordinates. Furthermore, it can introduce sources of variability prior of the device simulations. There are three variability sources from the SG: Random Discrete Dopants (RDD), Line Edge Roughness (LER) and Metal Gate Granularity (MGG), that can be considered individually or simultaneously.

The properties of semiconductor devices are dominated by quantum confinement and quantum transport phenomena, which must be taken into consideration in simulations together with charge and matter granularity. In addition, the simulation must include all geometric complexity such as surface transitions. Poisson module plays a central role in the modeling of the semiconductor device in NESS. A very important step in the quantum transport simulation of semiconductor devices working in strong confinement regime is the extraction of the effective masses for specific device cross section. NESS includes the EME module which allows the calculation of the effective masses, based on results from first principle band-structure simulation (Fig. 3). The EME module extracts the parabolic transport masses using parabola

☆ The review of this paper was arranged by Francisco Gamiz.

* Corresponding author at: Device Modelling Group, School of Engineering, University of Glasgow, Glasgow, Scotland, UK.
E-mail address: daniel.nagy@glasgow.ac.uk (D. Nagy).

https://doi.org/10.1016/j.sse.2022.108489

Available online 7 November 2022
0038-1101/© 2022 The Author(s). Published by Elsevier Ltd. This is an open access article under the CC BY license (http://creativecommons.org/licenses/by/4.0/).

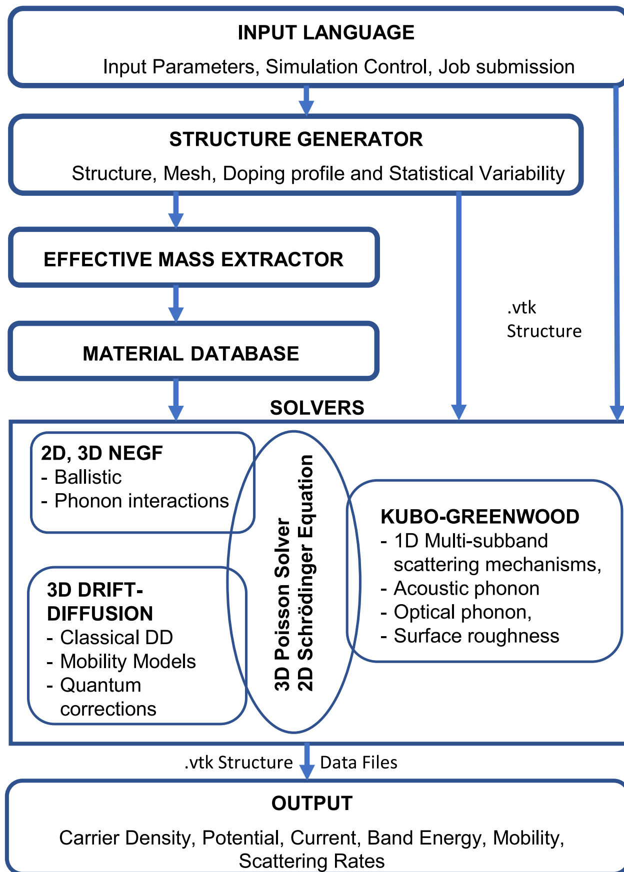

Fig. 1. Schematic modular structure of NESS.

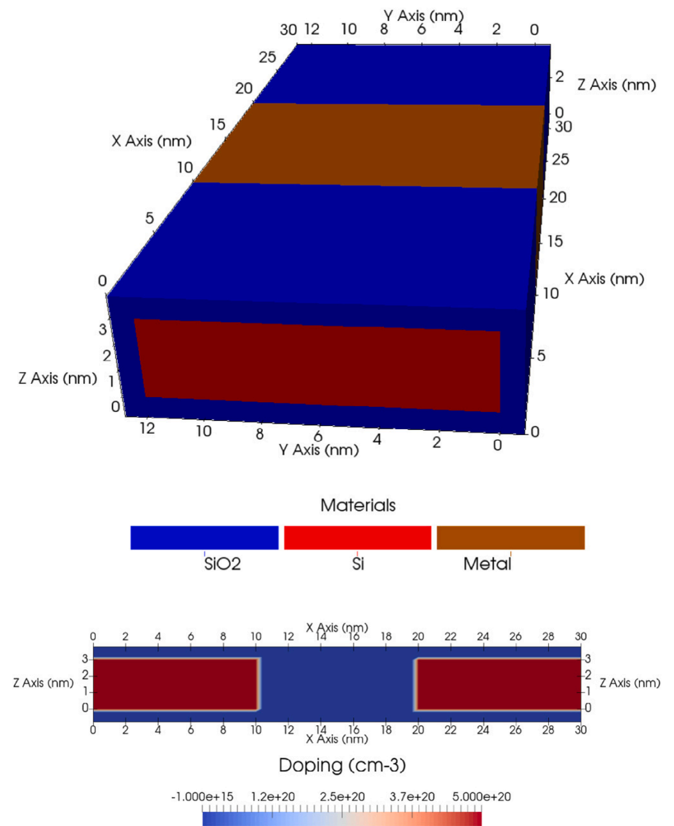

Fig. 2. Structure of nanosheet and doping profile along the channel.

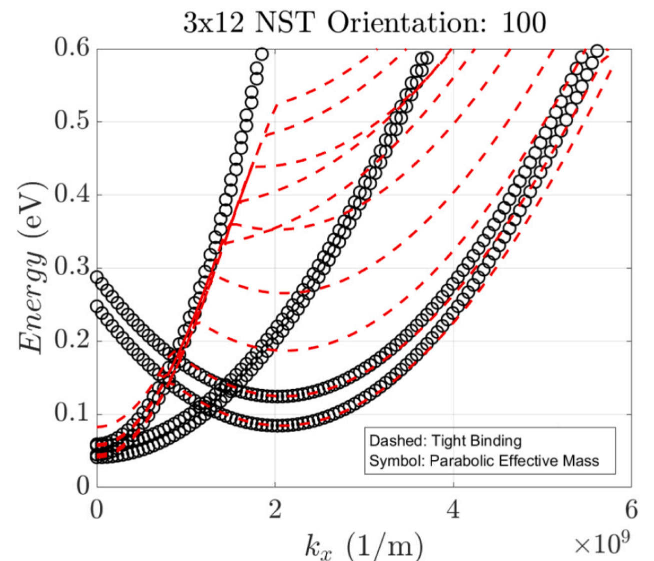

Fig. 3. Comparison of the electronic band-structure calculated using tight binding and the Parabolic Effective Mass approximation using the EME module for a 3 nm×12 nm Nanosheet with orientation along 100 direction.

fitting to the E-k relations for each sub-band and the confinement masses from the differences between the lowest sub-band energies.

The NEGF transport formalism provides a quantum treatment of electron transport to capture quantum phenomena such as tunneling, coherence, and particle–particle interactions in mesoscopic and nano-scale devices. We can simulate ballistic transport or can enable electron–phonon (e–ph) interactions within the self-consistent Born approximation by including the optical (Opt), acoustic (Ac), or optical–acoustic (Opt+Ac) e-ph scattering to study the transport in diffusive limit. The carrier density, potential profile, and the current are obtained by performing a self-consistent solution of the Poisson equation and the NEGF transport solver in coupled mode-space representation.

The DD module solves the carrier continuity equations self-consistently with the Poisson's equation. It includes different mobility models, including the doping dependence of the mobility (Masetti model [11]) and the transverse and longitudinal electric field dependence of the mobility (Yamaguchi [12] and Caughey–Thomas [13] models, respectively) to account for the impact of doping.

3. Results

SG — The structure generated for this paper is shown in Fig. 2. The device has a source/drain and gate length of 10 nm, a channel width and height of 12 and 3 nm, respectively. The gate oxide thickness is 1 nm SiO_2. For the current study we opted in using an ideal rectangular shape although a more realistic elliptical or circular cross section can be handled in NESS, for nanosheet and nanowire respectively.

Effective masses have a significant impact on quantum confinement, hence it is vital to be accounted in transport model simulations such as NEGF, and provide accuracy and realistic results. Fig. 3, shows the comparison of the tight binding band-structure obtained from the QuantumATK [14,15] and the parabolic extraction from the EME module of NESS [16], resulting to a very good agreement between the minima and curvature of the band-structure. The process of extracting the bulk effective masses, automatically prepares the material properties utilized by the solvers.

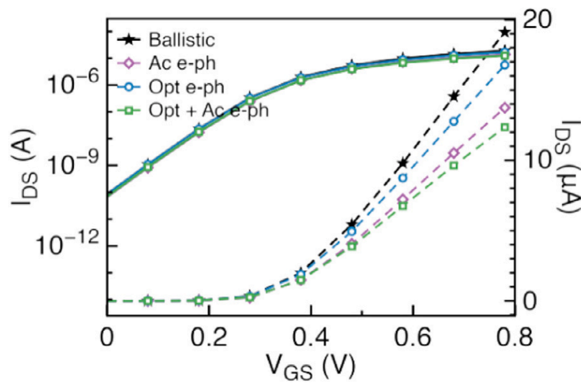

Fig. 4. I_D–V_G characteristics for ballistic and diffusive NEGF simulations at low drain (0.05 V) bias. The both linear and logarithmic scale have been depicted.

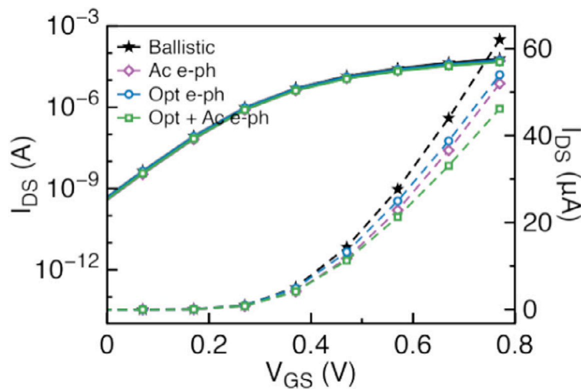

Fig. 5. I_D–V_G characteristics for ballistic and diffusive NEGF simulations at high drain (0.7 V) bias. The both linear and logarithmic scale have been depicted.

NEGF — The I_D–V_G characteristic at drain bias of 0.05 V, and 0.7 V are represented in Figs. 4, and 5, respectively. The effect of scattering is also demonstrated in the figures for acoustic, optical, and optical+acoustic electron–phonon interactions. The left, and right axis depict the drain current on logarithmic, and linear scale, respectively. As can be seen in the figures, level of accuracy of capturing the nanosheet threshold voltage highly depends on the utilized models. Inclusion of scattering reduces the current compared to the ballistic case, and the reduction becomes larger for higher gate biases. The possibility to individually turn on the scattering mechanisms allows us to study the effects and thus showing that the acoustic scattering limits the performance of the nanosheet the most. In Figs. 6, and 7 depict the OFF- and ON-state local density of states (LDOS), average potential, and energy sub-band structure computed along the nanosheet transport direction for low and high drain biases. As shown in the figures, the confined energy levels are pulled down by increasing the gate bias, i.e., going from the OFF-state (in ballistic limit) to the ON-state (in diffusive limit). This visualization, allows a deeper insight into the device physics governing the nanosheet.

DD — As shown in Fig. 8, the DD simulator can be calibrated to fit the NEGF results at low and high drain bias. This enables the use of classical DD simulator for situations where large number of simulations are needed e.g. in variability simulations where schemes like NEGF are computationally too expensive. The key parameters used for fitting the DD model are the gate workfunction and the mobility model parameters. Although not included in this abstract, in addition to classical DD simulator, NESS also incorporates quantum mechanical corrected version of DD using the Schrodinger equation based [17] and the density gradient method based [18] approaches which offer more realistic behavior than classical DD.

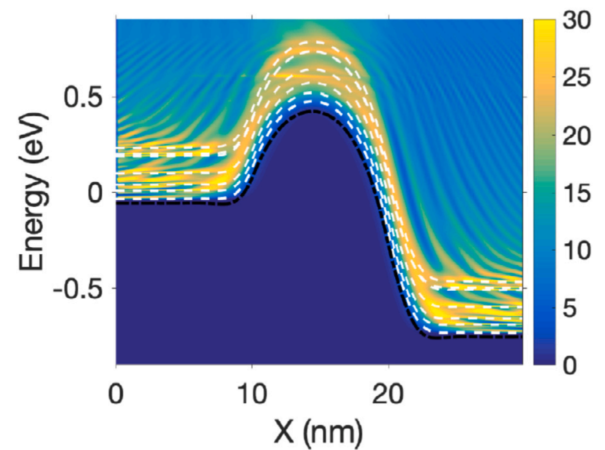

Fig. 6. The LDOS, average potential (black line), and energy sub-bands structure (white dashed lines) in the OFF-state in the ballistic limit along the nanosheet axis for V_D = 0.7 V and V_G = 0 V, and LDOS in units of eV^{-1}. Dark blue, and yellow indicates lower and higher LDOS magnitude, respectively. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

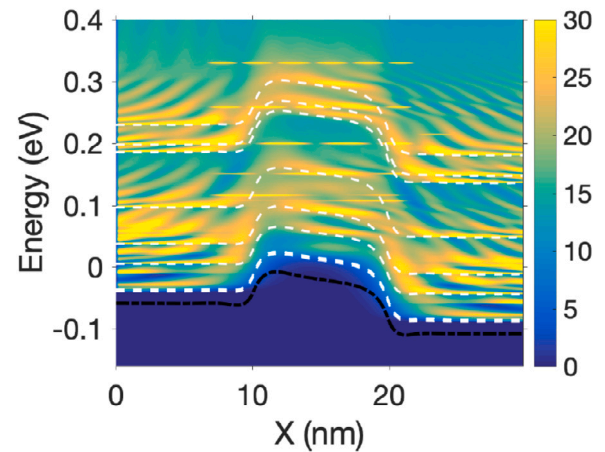

Fig. 7. The LDOS, average potential, and energy sub-bands structure in the ON-state with Opt+Ac electron–phonon scattering for V_D = 0.7 V and V_G = 0.7 V. The reference in energy is taken at the Source Fermi level (E_{FS} = 0 eV), and LDOS in units of eV^{-1}. Dark blue, and yellow indicates lower and higher LDOS magnitude, respectively. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

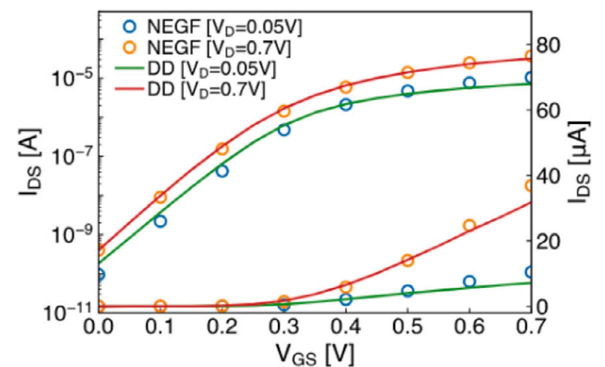

Fig. 8. Calibration of classical drift–diffusion simulator to NEGF results (with optical and acoustic phonon scattering) for I_D–V_G characteristics obtained at low and high drain bias.

4. Conclusion

In the current work we have successfully demonstrated the capabilities of NESS in the hierarchical predictive simulations of nanosheet transistors. The nanosheet transistor is at the center of both industry and academic research. We have carried out device simulations and showed that the more accurate NEGF simulations can be used for the calibration of the classical DD simulations within one single toolbox. Additionally we showed that the EME module can be used to extract the effective masses for confined structure like the nanosheet.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

References

[1] Bae G, Bae D-I, Kang M, Hwang S, Kim S, Seo B, et al. 3nm GAA technology featuring multi-bridge-channel FET for low power and high performance applications. In: 2018 IEEE international electron devices meeting. 2018, p. 28.7.1–4.
[2] Bufler FM, Jang D, Hellings G, Eneman G, Matagne P, Spessot A, et al. Monte Carlo comparison of n-type and p-type nanosheets with FinFETs: Effect of the number of sheets. IEEE Trans Electron Devices 2020;67(11):4701–4.
[3] Nagy D, Espiñeira G, Indalecio G, García-Loureiro AJ, Kalna K, Seoane N. Benchmarking of FinFET, nanosheet, and nanowire FET architectures for future technology nodes. IEEE Access 2020;8:53196–202.
[4] NESS, [Online]. Available https://www.gla.ac.uk/research/az/devmod/software/.
[5] Berrada S, Carrillo-Nunez H, Lee J, Medina-Bailon C, Dutta T, Badami O, et al. Nano-electronic Simulation Software (NESS): A flexible nano-device simulation platform. J Comput Electron 2020;19:1031–46. http://dx.doi.org/10.1007/s10825-020-01519-0.
[6] Medina-Bailon C, Dutta T, Rezaei A, Nagy D, Adamu-Lema F, Georgiev VP, et al. Simulation and modeling of novel electronic device architectures with NESS (nano-electronic simulation software): A modular nano TCAD simulation framework. Micromachines 2021;12(6). [Online]. Available https://www.mdpi.com/2072-666X/12/6/680.
[7] Dutta T, Medina-Bailon C, Adamu-Lema F, Rezaei A, Nagy D, Xeni N, et al. TCAD Simulation of novel semiconductor devices. In: 14th IEEE international conference on ASIC. 2021.
[8] Medina-Bailon C, Badami O, Carrillo-Nuñez H, Dutta T, Nagy D, Adamu-Lema F, et al. Enhanced capabilities of the nano-electronic simulation software (NESS). In: 2020 International conference on simulation of semiconductor processes and devices. 2020, p. 293–6.
[9] Medina-Bailon C, Dutta T, Adamu-Lema F, Rezaei A, Nagy D, Georgiev VP, et al. Nano-electronic simulation software (NESS): A novel open-source TCAD simulation environment. J Microelectron Manuf 2020;3:20030404.
[10] Rezaei A, Maciazek P, Sengupta A, Dutta T, Medina-Bailon C, Asenov A, et al. Statistical device simulations of III-V nanowire resonant tunneling diodes as physical unclonable functions source. Solid-State Electron 2022;194:108339, [Online]. Available https://www.sciencedirect.com/science/article/pii/S0038110122001113.
[11] Masetti G, Severi M, Solmi S. Modeling of carrier mobility against carrier concentration in arsenic-, phosphorus-, and boron-doped silicon. IEEE Trans Electron Devices 1983;30(7):764–9. http://dx.doi.org/10.1109/T-ED.1983.21207.
[12] Yamaguchi K. Field-dependent mobility model for two-dimensional numerical analysis of MOSFET's. IEEE Trans Electron Devices 1979;26(7):1068–74. http://dx.doi.org/10.1109/T-ED.1979.19547.
[13] Caughey DM, Thomas R. Carrier mobilities in silicon empirically related to doping and field. Proc IEEE 1967;55(12):2192–3. http://dx.doi.org/10.1109/PROC.1967.6123.
[14] Stokbro K, Petersen DE, Smidstrup S, Blom A, Ipsen M, Kaasbjerg K. Semiempirical model for nanoscale device simulations. Phys Rev B 2010;82(7):075420.
[15] Synopsys. QuantumATK version O-2019.12. 2019, [Online]. Available https://www.synopsys.com/silicon/quantumatk/.
[16] Badami O, Medina-Bailon C, Berrada S, Carrillo-Nunez H, Lee J, Georgiev V, et al. Comprehensive study of cross-section dependent effective masses for silicon based gate-all-around transistors. Appl Sci 2019;9(9). [Online]. Available https://www.mdpi.com/2076-3417/9/9/1895.
[17] Dutta T, Medina-Bailon C, Carrillo-Nuñez H, Badami O, Georgiev V, Asenov A. Schrödinger Equation Based Quantum Corrections in Drift-Diffusion: A Multiscale Approach. In: 2019 IEEE 14th nanotechnology materials and devices conference. 2019, p. 1–4. http://dx.doi.org/10.1109/NMDC47361.2019.9084010.
[18] Dutta T, Medina-Bailon C, Xeni N, Georgiev VP, Asenov A. Density gradient based quantum-corrected 3D drift-diffusion simulator for nanoscale MOSFETs. In: 2021 IEEE 16th nanotechnology materials and devices conference. 2021, p. 1–4.