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FRONTIERS IN ELECTRONICS

Advanced Modeling of Nanoscale Electron Devices

Editors
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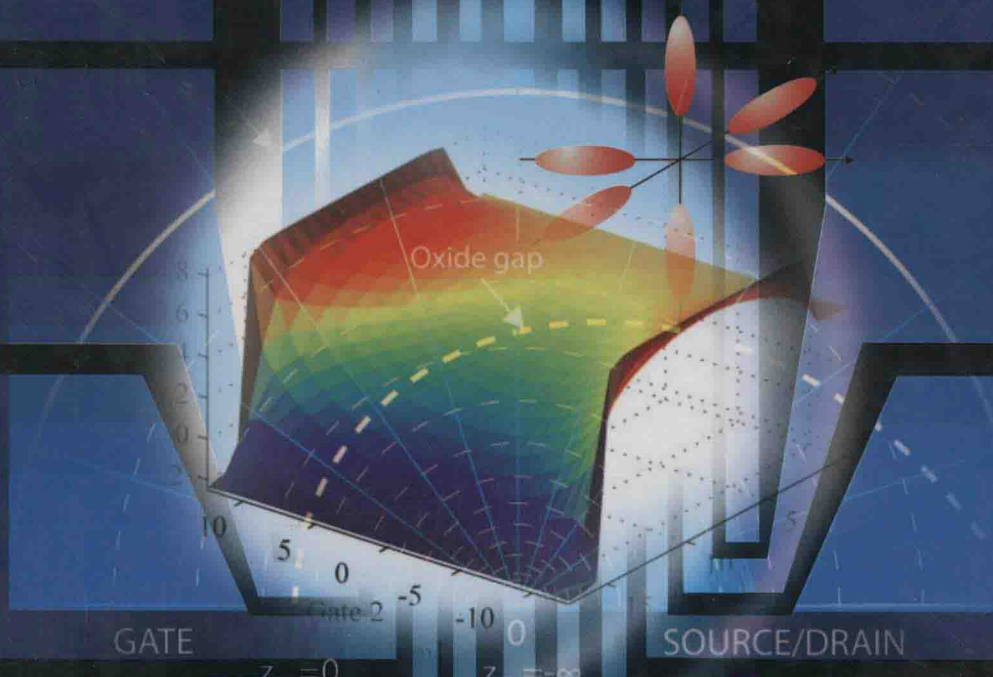

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Advanced Modeling of Nanoscale Electron Devices

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Advanced Modeling of
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SELECTED TOPICS IN ELECTRONICS AND SYSTEMS

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PREFACE

Accurate modeling of nanoscale electron devices is essential for both their technological improvement and optimization, and for their utilization in circuit design. Depending on the application, different levels of modeling have to be used. Technology oriented design requires highly physical models for both transport and electrostatics. Circuit design needs analytical compact models derived by considering a number of approximations.

This book on Advanced Modeling of Nanoscale Electron Devices, consists of four chapters to address at different modeling levels for different nanoscale MOS structures (Single- and Multi-Gate MOSFETs). The collection of these chapters attempts to provide a comprehensive coverage on the different levels of electrostatics and transport modeling for these devices, and the relationships between them. In particular, the issues of quantum transport approaches, analytical predictive 2D/3D modeling and design-oriented compact modeling are considered. It should be of interest to researchers working on modeling at any level, providing them with a clear explanation of the approaches used and the links with modeling techniques for either higher or lower levels.

List and short description of the chapters:

F. Gámiz, C. Sampedro, L. Donetti, A. Godoy, "Monte-Carlo Simulation of Ultra-Thin Film Silicon-on-Insulator MOSFETs"

This chapter reviews the basis of the Multi-Subband Monte Carlo (MSB-MC) method. In the first part of the chapter, the authors present a comprehensive coverage of the impact of different Buried OXide (BOX) configurations on the scaling of extremely thin fully depleted SOI devices using a Multi-Subband Ensemble Monte Carlo simulator (MS-EMC). In the second part of the chapter, the authors use the MS-EMC simulator to present a study of the electron transport in ultrashort DGSOI devices with different confinement and transport directions.

R. Clerc, G. Ghibaudo, "Analytical Models and Electrical Characterisation of Advanced MOSFETs in the Quasi-Ballistic Regime"

This chapter reviews the current understanding of the quasi-ballistic transport in advanced MOSFETs, underpinning the derivation and limits of corresponding analytical models. Furthermore, in order to estimate the "degree of ballisticity" achieved in advanced technologies, the chapter presents the different strategies used to compare these models and experiments.

T. A. Fjeldly, U. Monga, "Physics-Based Analytical Modeling of Nanoscale Multigate MOSFETs"

This chapter describes the derivation of a comprehensive modeling framework for double-gate and gate-all-around MOSFETs based on a conformal mapping analysis of the subthreshold potential distribution in the device body, and a self-consistent procedure in the above threshold regime. In an alternative modeling framework, covering a wide range of multigate devices in a unified manner, the potential distribution is derived from a select set of isomorphic trial functions that reflect the geometry and symmetry properties of the devices.

B. Iñiguez, R. Ritzenthaler, F. Lime, "Compact Modeling of Double and Triple Gate MOSFETs"

This chapter presents new techniques for the compact modeling of Double- and Triple-Gate MOSFETs. First of all, full analytical compact expressions for the charges and the drain current for each of the two channels of symmetrical Double Gate MOSFETs UTB SOI and Asymmetric Double Gate MOSFETs with independent gate operation are discussed. In the second part, the authors develop a framework for a fully 3D compact modeling of the electrostatics of Tri-Gate MOSFETs, including the back gate bias and short-channel effects. Finally, it further demonstrates that without the use of any fitting parameter, the model can be extended to nearly all the MuGFETs devices (GAA/ΠFETs/TGFETs/FinFETs/symDGFETs/FDSOI planar devices), and therefore could potentially be used as a core model for the scaling and calibration of a wide range of MuGFETs.

EDITORS
Benjamin Iñiguez
Tor A. Fjeldly

CONTENTS

MONTE-CARLO SIMULATION OF ULTRA-THIN FILM SILICON-ON-INSULATOR MOSFETs

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State-of-the-Art devices are approaching to the performance limit of traditional MOSFET as the critical dimensions are shrunk. Ultrathin fully depleted Silicon-on-Insulator transistors and multi-gate devices based on SOI technology are the best candidates to become a standard solution to overcome the problems arising from such aggressive scaling. Moreover, the flexibility of SOI wafers and processes allows the use of different channel materials, substrate orientations and layer thicknesses to enhance the performance of CMOS circuits. From the point of view of simulation, these devices pose a significant challenge. Simulations tools have to include quantum effects in the whole structure to correctly describe the behavior of these devices. The Multi-Subband Monte Carlo (MSB-MC) approach constitutes today's most accurate method for the study of nanodevices with important applications to SOI devices. After reviewing the main basis of MSB-MC method, we have applied it to answer important questions which remain open regarding ultimate SOI devices. In the first part of the chapter we present a thorough study of the impact of different Buried OXide (BOX) configurations on the scaling of extremely thin fully depleted SOI devices using a Multi-Subband Ensemble Monte Carlo simulator (MS-EMC). Standard thick BOX, ultra thin BOX (UTBOX) and UTBOX with ground plane (UTBOX+GP) solutions have been considered in order to check their influence on short channel effects (SCEs). The simulations show that the main limiting factor for downscaling is the DIBL and the UTBOX+GP configuration is the only valid one to downscale SGSOI transistors beyond 20 nm channel length keeping the silicon slab thickness above the theoretical limit of 5 nm, where thickness variability and mobility reduction would play an important role. In the second part, we have used the multisubband Ensemble Monte Carlo simulator to study the electron transport in ultrashort DGSOI devices with different confinement and transport directions. Our simulation results show that transport effective mass, and subband redistribution are the main factors that affect drift and scattering processes and, therefore, the general performance of DGSOI devices when orientation is changed

Keywords: Silicon-on-Insulator; scaling; short-channel effects; Multisubband Ensemble Monte Carlo; multigate transistor; quantum effects.

1. Introduction

New fabrication techniques and device concepts have been developed in the last 45 years to overcome the technological challenges that appear in order to follow Moore's Law and to fit the requirements of the International Technology Roadmap for the Semiconductor Industry (ITRS)[1]. Bulk MOSFET is still the main actor for the 32 nm node; however, as the channel length is reduced even more, short channel effects (SCEs) and variability problems arising from a highly doped channel[2] will make very difficult to maintain the standard bulk technology. In the search for the ideal device to be addressed for the 22 nm

node and beyond, different options are under study. One of the possibilities to overcome these issues is the use of multiple gate devices (MuGFETs) which are able to extend the end of the roadmap thanks to an outstanding SCEs control[3, 4]. Nevertheless, the decision of moving into 3D device architectures mass production is a real breakthrough and implies important efforts from an economical and a technological point of view. An intermediate solution, which has not been yet fully exploited, is to take advantage of the benefits that Silicon-On-Insulator (SOI) provides to planar technology. Among the main SOI features, we can highlight a better control of short channel effects, lower parasitic capacitance, and greater tolerance to radiation; moreover, all this is achieved while maintaining compatibility with existing silicon fabrication facilities. To the afore commented advantages of SOI technology, ultrathin Fully Depleted SOI (FDSOI) devices add a simpler fabrication process than in the standard technology, since some steps like HALO implants or recessed channel techniques are not necessary anymore. This fact allows a reduction in the overall cost and an almost straightforward layout transfer from bulk to SOI[5]. Single gate (SG) SOI structures are addressed for this solution since they can provide an extra control of SCEs, small V_{th} variability and a reduction in the leakage current. In SOI devices the channel is kept virtually undoped[6] minimizing the impact of random dopant fluctuations (RDF). In this way, the two main problems of bulk MOSFET technology for sub-32 nm technological nodes are overcome.

The real interest of the semiconductor community on SOI devices arises when the thickness of the silicon layer is reduced to the order of ten or less nanometers. From the simulation and modeling point of view, such ultra-thin SOI devices require the development of new scattering and transport models, because those used for bulk or for thick SOI devices where the two Si-SiO_2 interfaces can be de-coupled, must be modified. Novel effects, such as volume inversion[7] and sub-band modulation effect[8] appear, strongly modifying the scattering mechanisms, and therefore the carrier mobility. We have deeply studied during last years these effects in long channel devices (both n- and p-type channels). For extended reviews of the properties of electrons and holes in ultrathin SOI devices and see how they are affected by the silicon layer thickness and crystallographic orientation of the devices, the interested reader can check References 8-13 and references therein. In those works, we extensively showed that in ultra-thin SOI layers, carrier behavior is affected by the presence of the two potential barriers at the Si-SiO_2 interfaces. Electron wavelength in the confinement direction is comparable to the spatial confinement length: hence quantum effects are produced by both geometric and electric field confinement. Therefore, quantum effects are not only as important as in bulk inversion layers, but they also depend on silicon layer thickness and can give rise to novel effects such as volume inversion[7]. This phenomenon occurs when the distance between the potential wells at each interface is small and inversion carriers are not confined to one of the interfaces but are spread throughout the whole channel. This affects not only the total carrier density in the channel, but also, and notably, their distribution and, as a consequence, their scattering rates. Quantum effects are highly dependent on the confinement effective mass of carriers; therefore, they are strongly

affected by substrate crystal orientation. As a consequence, volume inversion effects change for different orientations and, clearly, depend on the type of carrier, i.e. electrons or holes. Figure 1 (left) shows the evolution of hole mobility with the silicon thickness in a DGSOI device, with different crystallographic orientations[13].

Certainly, the thickness of the silicon slab affects carrier distribution and carrier scattering, but we have also shown that phonon distribution in the structures is also strongly affected by the silicon thickness. Basically, there are two principal phenomena that modify the process of carrier scattering with the lattice vibrations in very thin silicon layers. First, the reduction of the electron momentum dimensionality and the momentum and energy conservation laws produces a drastic increase in the phonon scattering rate as the silicon thickness decreases[8]. The second phenomenon arises due to the modifications of the phonon modes caused by the acoustic and dielectric mismatches between the silicon and the silicon dioxide. These changes in properties give rise to confined and interface phonons in quantum wells, quantum wires and quantum dots[14]. The first phenomenon, increase in the phonon scattering rate in ultrathin silicon-on-insulator inversion produces a strong reduction in the mobility[10].To assess the second phenomenon we have developed a model to describe the quantization of acoustic phonon modes due to spatial confinement in silicon nanolayers using different structures and different boundary conditions[15,16]. Phonon quantization is included and the dispersion relations for distinct phonon modes are computed. This allows us to obtain the confined phonon scattering rates and to compute, using Monte Carlo simulations, the carrier mobility in ultrathin silicon on insulator inversion layers. We have shown that it is important to take into account acoustic phonon confinement in ultrathin silicon-on-insulator inversion layers by comparing electron mobility in ultrathin DGSOI devices, calculated assuming the usual bulk acoustic phonon model and also using the confined acoustic phonon model. Significant mobility reductions are obtained when the confined acoustic phonon model is used, even when other scattering mechanisms such as surface roughness scattering are taken into account. It is therefore essential to include such a model in the electron transport simulations of ultrathin SOI devices if we want to reproduce the actual behavior of electrons in silicon layers of nanometric thickness. Figure 1-(right) shows electron mobilities calculated by Monte Carlo simulation as a function of the silicon thickness in a double-gate SOI transistor at room temperature, taking into account the confined-phonon model.

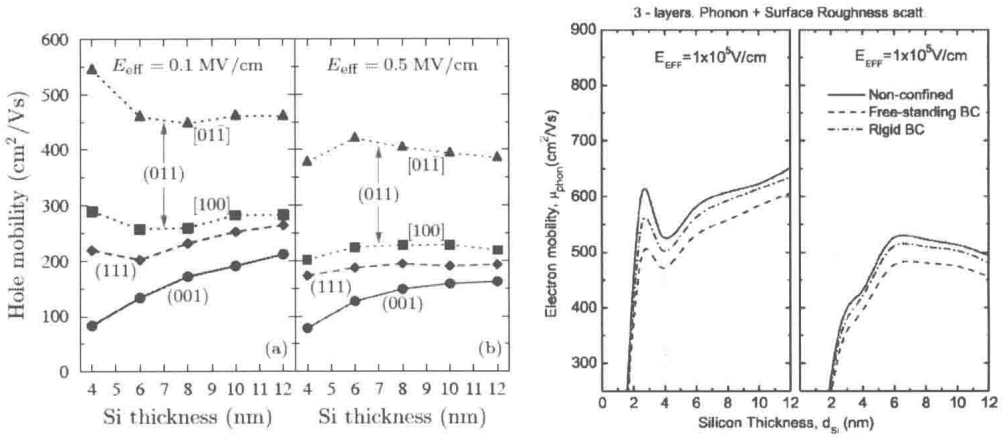

Fig. 1. (left) Effective hole mobility as a function of silicon thickness for different confinement and channel orientations (taken from Reference 13) (right) Monte-Carlo calculated electron mobility in double gate silicon-on-insulator inversion layers vs silicon thickness; surface roughness scattering has been taken into account in addition to phonon scattering (taken from Reference 15).

Up to now, we have considered the calculation of carrier transport properties in a boundless semiconductor structure, and therefore, we used a single particle Monte Carlo method. Thus we have showed the behavior of carrier transport in ultrathin SOI structures. However when we need to simulate the whole behavior of a realistic device, the single particle Monte Carlo approach is not appropriate because: i) the motion of particles is spatially restricted in the device region, so we need to set up suitable boundary conditions for the particles, and ii) the Boltzmann transport equation must be self-consistently solved with the Poisson and Schrödinger equations.

Different approaches from classical to full quantum can be considered depending on the needed accuracy, the computational resources and time available to perform the simulations. For the study of ultrashort channel devices, semi-classical approaches should not be used since confinements effects are of special importance[17]. At the opposite end of the spectrum, full quantum simulators based on numerical solutions of the Schrödinger equation or the Non-Equilibrium Green's Functions theory (NEGF) have also been developed[18]. In a quantum model, the transport of charged particles is treated coherently according to a quantum wave equation. In the simplest case of a single-particle Hamiltonian, carriers are considered as non-interacting waves described by the Schrödinger equation. The introduction of scattering in the simulations involves a very high computational cost and for this reason, only simplified models can be used in practical quantum simulations[18].

Between these extreme approaches, Ensemble Monte Carlo (EMC) simulators have been widely used since they present several advantages compared to full quantum approximations, such as a reduced computational cost, the possibility of considering a wide variety of scattering mechanisms and high accuracy. In order to include quantum effects in EMC codes, two main solutions are proposed in the literature. The first one

consists of adding a quantum term to the electrostatic potential in order to correct it. The aim of this correction is to mimic the electron concentration profile obtained when the Schrödinger equation is solved. The calibration of such corrections generally needs a set of fitting parameters (e.g. carrier effective mass in the density gradient model) but the results obtained are still accurate from the transport point of view for devices with silicon thicknesses as low as a few nanometers[19]. The most commonly used approaches include the Density Gradient[20], the Effective Potential[21], or the Multi-Valley Effective Conduction Band-Edge method (MV-ECBE)[22]. The second solution is obtained from the coupling of the Monte Carlo solution of the Boltzmann Transport equation and the 1D solution of the Schrödinger equation in the confinement direction, evaluated in different slices of the device. This method, the so-called Multi Subband Monte Carlo (MSB) approach[23,24,25,26] provides what is to date the most detailed description of carrier transport in the device, since the scattering rates are obtained from a quantum solution. In this review, we have used the Multisubband Ensemble Monte Carlo method to study:

(1) the possibilities that the combined use of Ultrathin Buried Oxide (UTBOX) and a ground plane (GP) offers to determine whether the scaling of ultrathin single-gate FDSOI devices is useful to fulfill the requirements of sub-32 nm nodes reducing the impact of thickness fluctuation effects.
(2) the orientation effects in ultra-short channel DGSOI devices.

2. Ensemble Monte Carlo simulators

Ensemble Monte Carlo (EMC) simulators are widely used since they present several advantages compared to full quantum approximations. A reduced computational cost, the possibility of considering a wide variety of scattering mechanisms and high accuracy for devices with silicon thicknesses as low as a few nanometers[19] are some of the advantages of such simulators. As mentioned above to include quantum effects in EMC codes, two are the main solutions proposed in the literature:

(1) The addition of a correction term to the electrostatic potential, i.e. quantum correction, to mimic the carrier concentration profile obtained when the Schrödinger equation is solved in the structure. Different models have been developed following this philosophy, giving a good accuracy-computational cost ratio. The most commonly used approaches include the Density Gradient[20], the Effective Potential[21] or the Multi-Valley Effective Conduction Band-Edge method (MV-ECBE)[22].

(2) The coupling of the Boltzmann Transport Equation (BTE) solved by the Monte Carlo method in the transport plane with the Schrödinger equation in the confinement direction evaluated in different slices of the considered device. This method, called Multi Subband Ensemble Monte Carlo approach (MSB-EMC)[23,24,25,26] provides what is to date the most detailed description of carrier transport in the device, since the scattering rates are obtained from a quantum solution.

In the following sections, the different EMC approaches to the quantum problem will be presented and compared.

2.1. *Quantum correction methods*

The easiest way to include quantum effects in semi-classical simulators such as EMC codes is by adding a correction term to the electrostatic potential obtained from the solution of Poisson's equation. These approaches are widely used in MC codes since the early 2000s due to their computational efficiency (close to their semiclassical counterpart) and good accuracy. However, the practical implementation needs, in general, a previous calibration to obtain the set of fitting parameters to obtain accurate results from the transport point of view.

2.1.1. *The effective potential method*

The effective potential model[21] obtains the corrected potential from the convolution of the electrostatic potential, $V(x_0)$, and a Gaussian function which represents the "effective size" of the particle. The one dimensional form of the correction is given by:

$$V_{eff}(x) = \frac{1}{\sqrt{2\pi}a_0}\int V(x')\exp\left(-\frac{(x-x')^2}{2a_0^2}\right)dx' \tag{1}$$

where a_0 represents the spreading of the wave-packet. The maximum of the carrier distribution is then shifted from the oxide interface, reproducing the total inversion charge. However, the charge profile results incorrect when is compared to the 1D Schrödinger solution[20]. Therefore, the method is not appropriate when magnitudes that depend on overlapping integrals involving envelope functions extracted from carrier distributions need to be calculated. This is the case of surface roughness models or inter-valley scattering rates when size quantization is taken into account.

2.1.2. *The density gradient method*

A better approximation obtained from the Wigner potential approximation is the Density Gradient (DG)[27]. This method, which is one of the first quantum corrections implemented on a simulation code, produces very good results especially in drift diffusion simulations. The correction term is given by the following expression:

$$V_q = 2b_n\frac{\nabla^2\left(\sqrt{n}\right)}{\sqrt{n}} \tag{2}$$

where

$$b_n = \frac{\hbar^2}{4r m_n^*} \tag{3}$$

$\hbar$ is the reduced Planck's constant, m_n^* represents the electron effective mass and r is a parameter whose value varies from 1 for pure states (low temperatures or very strong confinement) to 3 for mixed states (high temperatures or weak confinement). The last two parameters are used to fit the carrier profile to the obtained from the solution of the 1D Schrödinger equation.

Figure 2 shows a comparison of the electron concentration profile obtained from the solution of the Schrödinger equation (black), the Density Gradient approach (red) and the effective potential (blue) for a MOS structure[20]. As can be observed, although both approximated techniques fit the inversion charge, in the case of the Density Gradient, it is also possible to reproduce the inversion charge profile.

The drawback of density gradient approach is the difficult implementation of the model in EMC codes. The main reason is the dependence of the driving force with the third derivative of the carrier concentration which is a very noisy magnitude in EMC simulators. As a consequence, it is a hard task to obtain convergence and the corrections to the field should be calculated from different magnitudes trying to keep the accuracy of density gradient simulations.

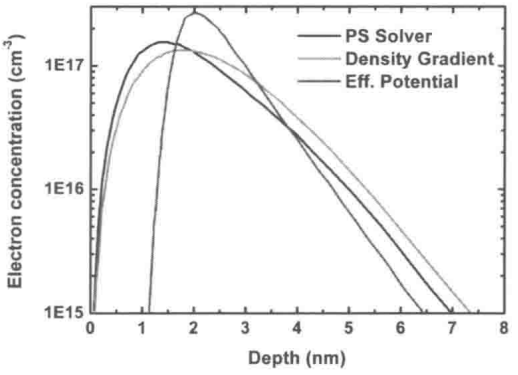

Fig. 2. Electron concentration profile obtained from the solution of the Schrödinger equation (black), the Density Gradient approach (red) and the effective potential (blue) for a MOS structure. As can be observed, the Density Gradient fairly reproduces the inversion charge profile [Reference 20].

2.1.3. *The effective conduction band edge (ECBE) method*

It is preferred, in MC simulations, to express the quantum correction in terms of the electrostatic potential, which is a smoother magnitude. The Effective Conduction Band-Edge method (ECBE) was developed to obtain the benefits of the density gradient in Monte Carlo simulations[28].

Starting from the density gradient, Eq (2), and assuming an exponential relation between the electron concentration and the effective potential, i.e.,

$$n \propto \exp\left(\frac{qV^*}{k_B T}\right) \tag{4}$$

the corrected potential V^* can be written as

$$V^* = V + V_q = V + \frac{q\hbar^2}{4 r m_n^* k_B T}\left(\nabla^2 V^* + \frac{q}{2k_B T}\left(\nabla V^*\right)^2\right) \tag{5}$$

The equation is solved in a self-consistent way with Poisson's equation and the BTE using the boundary conditions proposed by Jin et al.[29]. Depending on the device geometry (Figure 3-(left)) and bias point, the population of the different valleys may change. As a consequence, there is a variation in the confinement effective mass when only one valley is considered which has to be taken into account to reproduce the charge profile obtained from the solution of the 1D Poisson-Schrödinger system. The practical consequence is the use of the effective mass as a fitting parameter, as shown in Figure 3-(right). To avoid this issue, an improved version of the ECBE was developed to take into account the effect of different valleys and the orientation effects on the device performance.

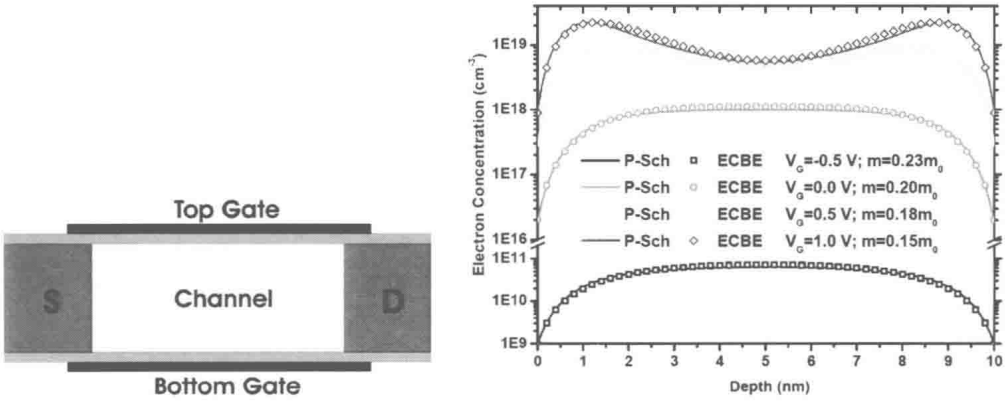

Fig. 3. (left) Double gate Silicon-on-insulator structure used in the simulations. (right) Poisson-ECBE and Poisson-Schrödinger solutions of the electron concentration in a 10 nm thick DGSOI structure for different gate bias. The ECBE approach gives a very good fit with the results obtained from the quantum calculations. However it is necessary to fit the effective mass for each bias condition.

2.1.4. *The multivalley effective conduction band edge approach (MV-ECBE)*

The standard ECBE method gives very good results when studying different SOI structures[22]. However, the main problem with this approach comes from the use of the effective mass as a fitting parameter. Nowadays, the study of SOI devices with