Numerical Analysis on Core-Shell Based GeSi Nanowire MOSFETs

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ABSTRACT

This paper investigates the transport properties of the core-shell based silicon/Germanium nanowire MOSFETs by a numerical method. Coupling Poisson's equation to Schrödinger's equation for electrostatics calculation, and electron structure to current transport equation for channel current computation, the electronic structure, quantized energy levels, relevant wave functions and charge distribution are solved self-consistently by a finite numerical method. Based on these findings, the transistor performances, including the capacitance characteristics and drain current, are further predicted.

Keywords: Non-classical MOSFETs; Device physics; with core-shell GeSi nanowire MOSFET.

1 INTRODUCTION

With the scaling of transistors to the 32nm regime, it has been anticipated that conventional scaling approach will soon hit the limit [1]. To continue the scaling trends for nano-electronic technologies, nanotubes and nanowire are considered as alternatives to conventional metal-oxide-semiconductor field-effect transistors (MOSFETs) [2] due to their unique one-dimensional electronic structure to reduce short-channel-effects (SCE) and scattering of conducting carriers. In particular, the symmetric concentric structure of nanowire created a cylindrical symmetry that is different from other structures being pursued in the industry like FinFET [3] and Trigate MOSFETs [4]. Many popular effects such as carrier confinement, strain and stress in these kinds of transistors would have a concentric dependence rather than the planar coordinate structure.

In particular, heterostructures with Ge/Si core/shell nano-wire [5] has been demonstrated to provide "hole gas" with high mobility at its Ge core that give rises to a high performance p-channel like FETs. The concentric nanowire structure has the potential to provide superior performance compared with other nano-transistor structures. However, the transport mechanism in the concentric nanowire transistors is not clear due to the lack of understanding on the detailed physics that govern their behavior. In addition, there is no design tool for simulation. This prevents the evaluation when these nanowire transistors are used in actual circuit. The study of high-performance nanowire FETs has also been hindered by difficulties in producing uniform nanowire in a top-down approach with controllability and reproducibility. In this work, we propose a detailed numerical study on the device physics that govern the transport mechanism of Silicon/Germanium nano-wire transistors with the core-shell structure and evaluate the transistor performance from the self-consistent numerical solutions between the electrostatics, carrier refinement, and the current transport.

2 NUMERICAL APPROACH

Conduction in the nanowire transistor is governed by 2-D quantum mechanical confinement, which determines that conventional modeling approach that based on Charge-Sheet Approximation cannot be used. Fortunately, the symmetrical properties of concentric nanowire structures simplify the boundary conditions so that the solution of Poisson equation and Schrödinger equation can be expressed in one-dimensional form. As a result of a previous research in our group, a quantum simulator based on the solution of Poisson equation and Schrödinger equation has already been developed [6]. This tool will be extended to model the effects of electron wave function penetrations through the multiple layers in the concentric nanowire structures. The numerical results will serve as a verification tool to the characteristics and performance of the nanowire MOSFETs with the core-shell structure.

In the theoretical formulation, we have two main equations: Schrödinger and Poisson equations, each will be later turned into discrete format for the finite element method. Basic transport equations including current density equation, continuity equation and Einstein relation are also involved. As is discussed above, the simplification resulting from symmetrical properties of this SiGe nanowire MOSFETs with core-shell structure leads to a one-dimensional continuous Schrödinger equation:

$$\left(-\frac{\hbar^2}{2}\frac{d^2}{dx^2}\frac{1}{m(x)}+qU(x)\right)\cdot\Psi_i(x)=E_i\cdot\Psi_i(x), i=1,2,3,.....,N \quad (1)$$

where the effective mass $m(x)$ is taken as energy-independent and lposition-dependent.

In order to apply the finite element method to Eq.(1), this equation is turned into a discrete form using central difference method [7]:

$$\frac{-\frac{\hbar^2}{2}\cdot\frac{\Psi(x_{k-1})}{m^-(x_k)}}{\Delta x_{k-1}\cdot\overline{\Delta x_k}}+\left[\frac{\hbar^2}{2}\cdot\frac{\frac{1}{m^+(x_k)}}{\Delta x_k\cdot\overline{\Delta x_k}}+\frac{\hbar^2}{2}\cdot\frac{\frac{1}{m^-(x_k)}}{\Delta x_{k-1}\cdot\overline{\Delta x_k}}+q\cdot U(x_k)\right]\cdot\Psi(x_k)-\frac{\frac{\hbar^2}{2}\cdot\frac{\Psi(x_{k+1})}{m^+(x_k)}}{\Delta x_k\cdot\overline{\Delta x_k}}=E\Psi(x_k) \quad (2)$$

where:

$$m^-(x_k)=\frac{1}{2}[m(x_{k-1})+m(x_k)],$$

$$m^+(x_k)=\frac{1}{2}[m(x_k)+m(x_{k+1})],\ \overline{\Delta x_k}=\frac{1}{2}[\Delta x_{k-1}+\Delta x_k]$$

Similarly, the initial form of one-dimensional continuous Poisson equation is expressed as:

$$\frac{d}{dx}[\varepsilon(x)\cdot\frac{d}{dx}U(x)]=-\rho(x) \quad (3)$$

where $\rho(x)$ is the charge density.

Change it into discrete form:

$$U(x_{k-1})\cdot\frac{\varepsilon_{k-0.5}}{\Delta x_{k-1}\cdot\overline{\Delta x_k}}-U(x_k)\cdot[\frac{\varepsilon_{k-0.5}}{\Delta x_{k-1}\cdot\overline{\Delta x_k}}+\frac{\varepsilon_{k+0.5}}{\Delta x_k\cdot\overline{\Delta x_k}}]+U(x_{k+1})\cdot\frac{\varepsilon_{k+0.5}}{\Delta x_k\cdot\overline{\Delta x_k}}=-\rho(x_k) \quad (4)$$

where: $\varepsilon_{k-0.5}=\frac{1}{2}[\varepsilon(x_k)+\varepsilon(x_{k-1})],\ \overline{\Delta x_k}=\frac{1}{2}[\Delta x_{k-1}+\Delta x_k]$

Based on the Fermi-Dirac distribution, the quantized carrier distribution is calculated by:

$$n(x)=\int g(E)\cdot f(E)dE=\sum_{l,k}f_0(\varepsilon_l,k_z)\cdot|\Psi(x)|^2$$
$$=\sum_l g_l\cdot\left(\frac{\sqrt{2m(x)kT}}{2\pi\hbar}\cdot\int_0^{\infty}\frac{\varepsilon^{-\frac{1}{2}}}{1+\exp(\varepsilon-\xi)}d\varepsilon\right)\cdot|\Psi(x)|^2,\ \xi=\frac{E_F-\varepsilon_l}{kT} \quad (5)$$

From Eq.(5), we have

$$\therefore n(x_k)\approx\sum_l g_l\cdot\left(\frac{\sqrt{2m(x_k)kT}}{2\pi\hbar}\cdot\int_0^{15000}\frac{1}{1+\exp(\varepsilon^2-\xi)}d\varepsilon\right)\cdot|\Psi(x_k)|^2 \quad (6)$$

where $\xi=\frac{E_F-\varepsilon_l}{kT}$

Here the upper limit of 15000 is an approximation to substitute for $+\infty$ in the accurate expression of the integral. Since the function: $f(\varepsilon)=\frac{1}{1+\exp(\varepsilon^2-\xi)}$ approaches zero much quicker than the function: $f(\varepsilon)=\frac{1}{\varepsilon^2}$ does when ε approaches $+\infty$, this approximation is ideal, which has also been proved by computational experiments.

Based on the charge conservation concept, the total charge in the space charge layer is written as:

$$\rho(x_k)=q\left[p(x_k)-n(x_k)+N_D^+(x_k)-N_A^-(x_k)\right] \quad (7)$$

By solving Eq.1-4 numerically using a self-consistent method [8] that includes two solvers, one for Poisson solution for the set-up of initial guess of potential distribution, and the other for potential distribution with the knowledge of electron concentration as a function of position after it is derived from the Schrodinger solver, we can get $p(x_k)$, $n(x_k)$, $\Psi(x_k)$, $U(x_k)$ and $E(x_k)$ so as to calculate the drain current.

The current can be calculated by applying current continuity equation. Supposing that the electron mobility is a constant, according to Pao-Sah equation [9], the discrete form of current density equation is:

The corresponding discrete form is:

$$I_{ds}=\frac{\mu_n W q_0}{L}\sum_k n(V_k)V_k(A) \quad (8)$$

where $n(V_k)$ is the bulk electron distribution derived from the linear electron carrier distribution calculated in Eq.(6) by dividing it with the unit area applied in the discrete coordinate system. Here μ_n is viewed as a constant in this presented model for simplification. Later we would depend on Eq.(8) to simulates the electrical characteristics of this presented model with core-shell structure.

3 RESULTS AND DISCUSSION

For the studied nanowire structure to be recognized for its anticipated electrical applications, a clear view of energy band structures, wavefunctions and energy levels is indispensable and is thus obtained first. For simplification we assume that there are no interface states at the boundaries of the materials. Shown in Fig.1-2 are the results of electron wave functions computed from a 1-D Si/Ge nanowire MOSFEET model with core-shell structure, with a silicon radius (R_{Si}) of 10nm, a germanium radius (R_{Ge}) of 5nm and a gate oxide thickness (T_{ox}) of 2nm, under different gate voltages. Actually the energy level degenerates into many subbands. For instance, in the case of a gate voltage of 0V, there are 16 and 5 subbands for heavy and light electrons respectively. However, since only the wavefunctions of the first few energy levels are comparatively significant, the rest are not shown in Fig.1-2. As to the case where V_{gs}=0V, only the first 6 of heavy electron wave functions and the first 3 of light electron wave functions plotted, as is shown in Fig.1a. From this series of wavefunctions versus gate voltage profiles, it is clear that the gate voltage (V_{gs}) has a powerful control over the electron distributions: while the effective V_{gs} approximates zero, there are several wavefunctions in the similar orders. When the effective V_{gs} increases, only one or two wavefunctions stand out and all the other wavefunctions are overwhelmed. This agrees with the device physical theory that electrons are attracted and trapped in the quantum well in the inversion layer under a high positive gate voltage, thus forming an electron-dominated channel. The higher the gate voltage, the higher are the electron concentrations in the inversion layer and the nearer the peaks to the semiconductor surface. Since the induced electrons distribute in several sub-energy levels to result in the current transport, such a split distribution on the number of energy bands, that is, a limitation on conduction channels, can benefit electrical performance through a reduction in scattering [10].

Fig.3 illustrates the comparison of electron concentration distributions with and without quantum mechanical effect (QME) and for different R_{Ge} with the same gate voltage and R_{Si}-R_{Ge}; different parameter Rsi-R_{Ge} with the same R_{Ge} and different R_{Ge} changing with the same R_{Si}. It is concluded from these figures that the classical device physics excluding QME predicts an electron distribution with sharp peak very close to the semiconductor surface. In contrast, the quantum based

physics picture demonstrates that the electron concentration peaks always have a distance from the semiconductor surface. It is very interesting that the electron distribution shows two peaks either in the classical or the quantum physics picture, which will benefit the channel current transport. This is why the core-shell structure of SiGe nanowire has a series transport advantages over the traditional nano-wire structure. On the other hand, such distribution characteristics also explain why the charge-sheet approximation is no longer suitable for the calculation of drain current in a nanowire MOSFETs, as the quantum mechanical effect is no longer negligible. Moreover, it is also found that the peak of the surface electron concentration also increases with the increase of the silicon radius.

Last but not the least, it seems that the slight variance of R_{Ge} does not affect the electron distribution much, especially that in the quantum well of the channel. This indicates that SiGe nanowire MOS capacitance is not very sensible to the proportion of R_{Si}-R_{Ge} to R_{Ge}, as long as the whole semiconductor layer thickness remains. Also, it reveals the inefficacy of the charge-sheet approximation in nanowire device.

The conductance band profile is plotted in Fig.4 for the gate voltage of 2V. Compared with the case of the zero gate voltage, it is observed from Fig.4 that the quantum well becomes shallower slightly, and its depth decreases significantly from 3.15V to 1.39V. It is also observed that the height of the barrier at the interface between Si and Ge also lowers slightly from 0.5 V to 0.37V. This result coincides with the increase of electron concentration when a gate voltage of 2V is applied to the SiGe nanowire MOSFETs.

Fig.5 plots the capacitance characteristics of a core-shell nanowire MOSFET. It is observed that the core-shell SiGe nanowire MOSFET capacitance presented here has a near-static capacitance characteristic resembling that of a classical bulk MOSFET very much, in that both have a depletion region where the capacitance increase with the increasing V_{gs}, and a strong inversion region where the gate capacitance approaches saturation with the increase in V_{gs}. These characters suggest similar capacitive applications of the presented model to those of a bulk MOSFET in the integrated circuit.

Fig.6 plots the numerical I_{ds}-V_{ds} curves, compared with the classical model without quantum mechanical effects, while Fig.7 depicts the I_{ds}-V_{gs} curves calculated from Eq.(8) for different combinations of R_{Si} and R_{Ge}. These figures show that all the drain current curves, either from the quantum based transport or the classical device physics, share the clear separation of three operation regions: the subthreshold, the linear and the saturation region. However, it seems that the quantum based transport can carry out a larger channel current than the classical one. This accords with the observed high performance of SiGe nano heterostructures. [11-12] Last but not the least, I_{ds} rises with the rise of either (R_{Si}-R_{Ge}) or R_{Ge}. All these findings imply the methods of controlling the drain current by geometry parameters.

4 CONCLUSIONS

In summary, the characteristics and performance of the SiGe nanowire MOSFET with core-shell structure has been studied in this paper by solving the Poisson-Boltzmann equation and the Schrodinger Equation self-consistently, coupled to the channel carrier transport equation. The energy band and the wavefunctions are obtained first, and then analyzed in details, followed by the study of the drain current characteristics and gate capacitance. It is shown how the quantum mechanical effects and different geometry combinations of R_{Si} and R_{Ge} affect the micro electron energy level, carrier distribution and the macro channel current transport. All these provide a useful result for the device engineers how to design and optimize the performance of the SiGe nanowire MOSFET with core-shell structure for the beyond 10nm generation integrated circuit application.

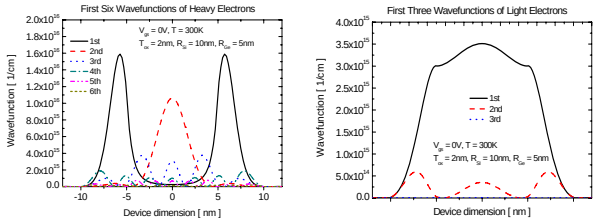


Fig.1 First few wavefunctions of heavy electrons and light electrons of SiGe Nanowire MOSFET while V_{gs}=0V.

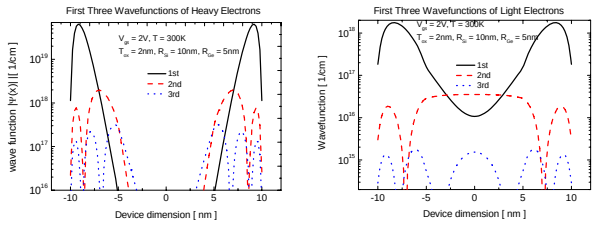
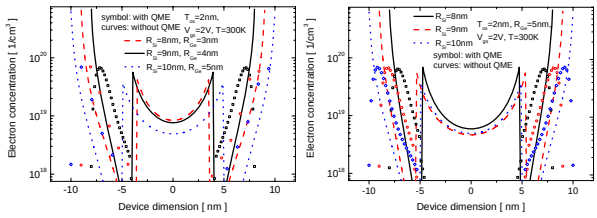


Fig.2 First few wave functions of heavy electrons and light electrons of SiGe Nanowire MOSFETs while V_{gs}=2V.



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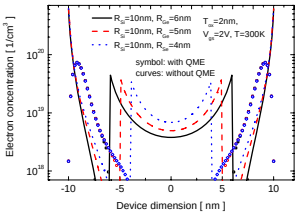

Fig.3 The comparison of electron concentration distribution along the vertical direction with and without QME for different combination of RSi and RGe.

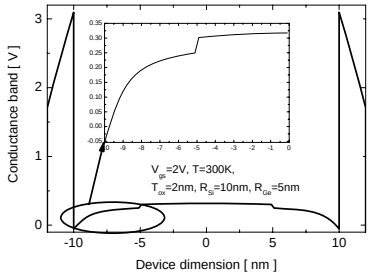

Fig.4 The conductance band profile along the vertical direction of SiGe nanowire MOSFETs with V_{gs}=2V.

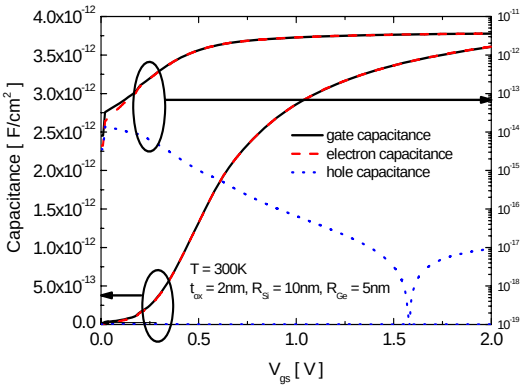

Fig.5 gate capacitance, electron capacitance and hole capacitance versus gate voltage.

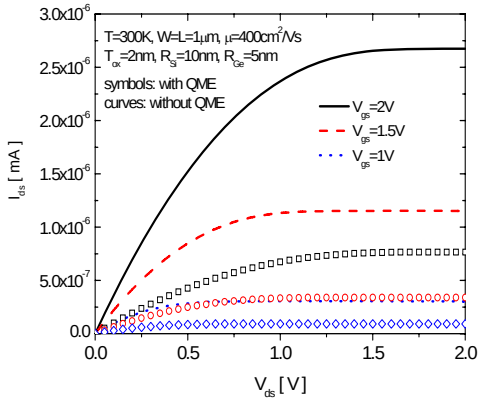

Fig.6 I_{ds}-V_{ds} curves with R_{Si}=10nm, R_{Ge}=5nm.

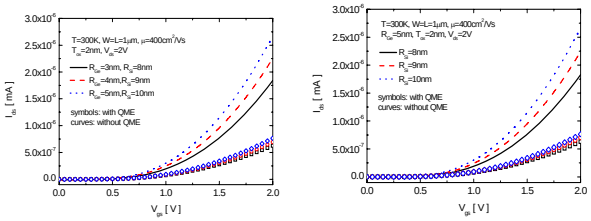

Fig.7 Ids-Vgs curves of different RGe and the same RSi-RGe, of different RSi-RGe and the same RGe.

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