Università di Pisa

Technique and Methods for the Simulation of nanoscale ballistic

Giuseppe Iannaccone

Dipartimento di Ingegneria dell'Informazione: Elettronica, Informatica, Telecomunicazioni, Università di Pisa

Gianluca Fiori

Dipartimento di Ingegneria dell'Informazione: Elettronica, Informatica, Telecomunicazioni, Università di Pisa

Gilberto Curatola

Dipartimento di Ingegneria dell'Informazione: Elettronica, Informatica, Telecomunicazioni, Università di Pisa

Techniques and methods for the simulation of nanoscale ballistic MOSFETs

G. Iannaccone*, G. Fiori, G. Curatola

Dipartimento di Ingegneria dell'Informazione, Università degli studi di Pisa,
Via Diotisalvi 2, I - 56122 Pisa, Italy   *e-mail: g.iannaccone@iet.unipi.it

ABSTRACT — **In this paper, we present the methods and the techniques we use for performing the simulation of nanoscale ballistic MOSFETs in bulk silicon, silicon on insulator, and silicon-germanium. Results for typical structures with channel length of 25 nm are presented.**

I. INTRODUCTION

In sub-100 nm MOSFETs a significant fraction of electrons contributing to the drain current traverse the channel without suffering inelastic scattering. This fraction of "ballistic" electrons is expected to increase in the next generation of CMOS devices [1], and to predominate over electrons undergoing phonon scattering in devices with channel length shorter than 30 nm [2]. Proper simulation tools of nanoscale MOSFETs must therefore be able to take into account "ballistic" electrons not just as a perturbation to a "normal", quasi-thermal electron distribution, but as mainstream electrons, and, on the contrary, to consider thermalized electrons with a perturbative approach. Simulations of completely ballistic MOSFETs have already been proposed, based on semiclassical Monte Carlo codes [3] and on a scattering theory of MOSFETs [4], and exhibit significant differences with respect to simulations based on drift-diffusion or energy balance models.

However, nanoscale MOSFETs also have other peculiar properties that can only be reproduced with a quantum simulation: the strong vertical confinement causes a large separation between the two-dimensional subbands in the channel, so that typically only the first subband is populated, and the threshold voltage is significantly larger than the value obtained from a naive semiclassical simulation. In addition, the degree of confinement depends on the charge profile, which in turn depends on the continuity equation, and therefore requires the self-consistent solution of device equations.

In recent years, MOSFETs realized with strained silicon channels on relaxed SiGe substrates have been proposed for improving high frequency and low power characteristics. Also in this case, the strained silicon layer has a thickness of the order of a few nanometers, and therefore causes significant quantum confinement of electrons in the channel. It is well known that electron mobility in strained silicon is significantly larger than in bulk silicon: it is therefore important to understand whether strained silicon provides comparable advantages also in the ballistic regime, when mobility has no physical meaning.

II. MODEL

In this paper we present a code for the two-dimensional simulation of ballistic MOSFETs, in which quantum confinement in the channel is properly taken into account, and electrons are assumed to conserve energy while they traverse the channel. The code is based on the self-consistent solution in two dimensions of the Poisson equation, of the Schrödinger equation, and of the continuity equation for ballistic electrons. The details of the model have already been described in [5] and [6] and will be only mentioned here.

Here, we want to discuss in some detail the choice of the occupation factor of electron states traveling from the source to the drain and viceversa, since a proper choice of such occupation factor, by itself, guarantees that the continuity equation for the ballistic current be obeyed (this is a great advantage, since there is no additional equation to be solved except Poisson-Schrödinger).

Let us consider the situation sketched in Fig. 1: the first subband profile in the longitudinal direction (from source to drain) has a peak close to the middle of the channel. This peak represents the energy of the barrier controlling the drain current: the maximum value of the subband (let us call it E_{sbmax}) is modulated via the gate voltage. If we assume that electrons do not lose energy, then we can assign to each electron state the occupation factor corresponding to the originating contact. Let us call $f(y,E)$ the occupation factor at coordinate y (in the longitudinal direction) and for energy E. If $E < E_{sbmax}$ then $f(y,E) = f_{FD}(E_{FS},E)$ if y is on the left of the peak, $f(y,E) = f_{FD}(E_{FD},E)$ if y is on the right of the peak. f_{FD} is the Fermi-Dirac occupation factor, E_{FS} and E_{FD} the Fermi energy of the

source and drain reservoirs, respectively. Instead, if $E >$ E_{sbmax} , then for each y and E there is a state traveling towards right (originating from the source) and a state traveling towards left (originating from the drain), therefore, the occupation factor is $f(y,E) = [f_{FD}(E_{FS},E) + f_{FD}(E_{FD},E)]/2$.

If we consider only the first subband E_{sb}, associated to the eigenstates $\Psi_i(x,y)$ obtained by solving the Schrödinger equation in the vertical direction with the longitudinal effective mass, the electron density n reads:

$$n(x,y) = |\Psi_i(x,y)|^2 \int_0^{E_{sbmax}-E_{sb}(y)} D_i(E_y) f_{FD}(E_{FS}, E_y + E_{sb}(y)) dE_y$$

$$+ |\Psi_i(x,y)|^2 \int_{E_{sbmax}-E_{sb}(y)}^{\infty} D_i(E_y)$$

$$\times \left[\frac{f(E_{FS}, E_y + E_{sb}(y)) + f(E_{FD}, E_y + E_{sb}(y))}{2} \right] dE_y$$
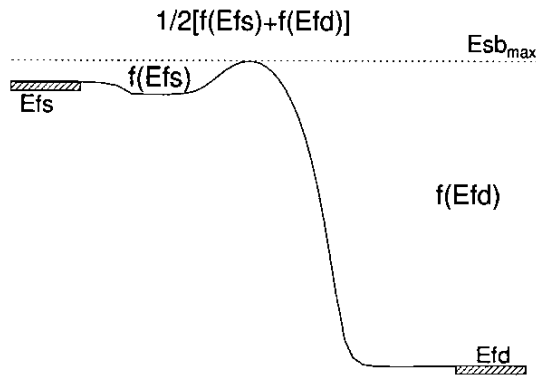
$$1/2[f(Efs)+f(Efd)]$$

Fig. 1: Sketch of the subband profile along the channel, and of the occupation factor assigned to electron states as a function of energy and position.

where $D_i(E_y)$ is the longitudinal density of states.

The ballistic current density in a subband, per unit width, is given by the formula

$$J_i = q\Gamma(1/2) \frac{\sqrt{2m_i kT}}{h^2}$$

$$\int_{E_{sbmax}-E_{sb}}^{\infty} \left[F_{-1/2}\left(-\frac{E_{sb} + E_y - E_{FS}}{kT} \right) - F_{-1/2}\left(-\frac{E_{sb} + E_y - E_{FD}}{kT} \right) \right] dE_y$$

where $F_{-1/2}$ is the Fermi integral of order $-1/2$. The total current is obtained by summing up the above expression over all subbands.

In addition, our code takes properly into account the effect of strain on the band structure of silicon and on ballistic transport in the channel, using a model described in Ref. [7].
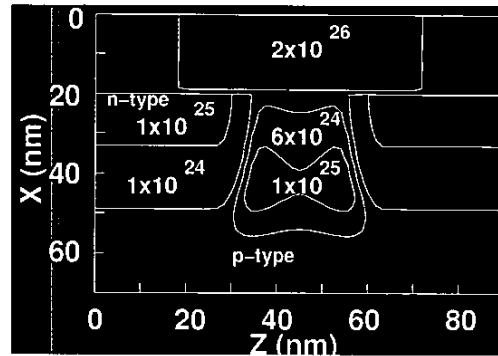

Fig. 2: Doping profile of the 25 nm well tempered MOSFET, with super-halo doping, proposed by D. Antoniadis [5]
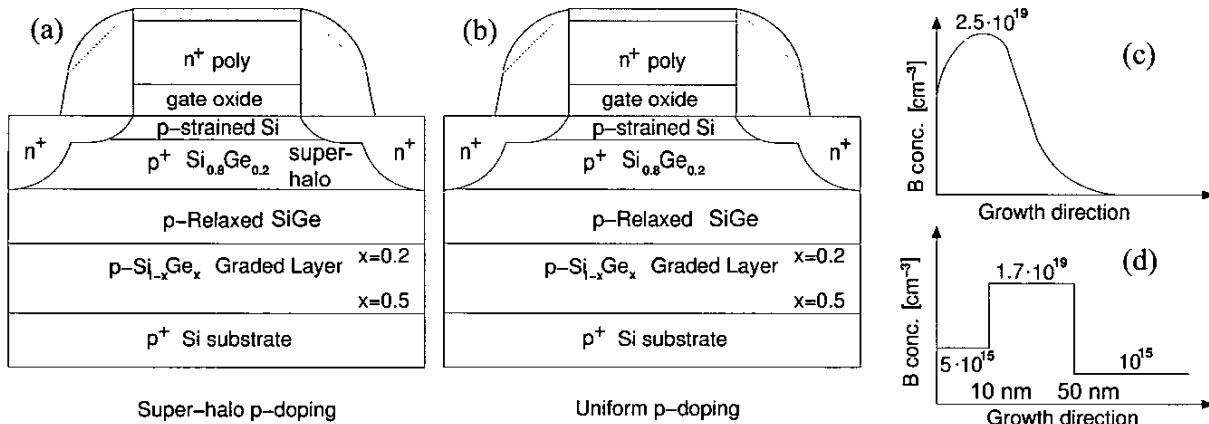

Fig. 3: SiGe MOSFETs considered (not in scale): Strained-Si MOSFET(a) with super-halo p doping (c); Strained-Si MOS with epitaxial SiGe p-doped layer (b)(d).

Here, we apply the code to the simulation of three different types of devices:

- a bulk-Si MOSFET with channel length of 25 nm and super-halo p-doping, proposed by D. Antoniadis as a benchmark device [8] (doping profiles are shown in Fig. 2);
- a strained-Si MOSFETwith the same doping profile shown in Fig. 1, fabricated on the SiGe heterostructure shown in Fig. 2 (on the left). The strained silicon layer is 10 nm.
- a strained Si MOSFET with an epitaxial SiGe p-doped layer instead of the implanted super-halo p doping on the layer structure shown in Fig. 3 (right). The strained silicon layer is 10 nm, the p-doped epitaxial SiGe layer is 40 nm, with $N_A = 1.7 \times 10^{19} \text{cm}^{-3}$.
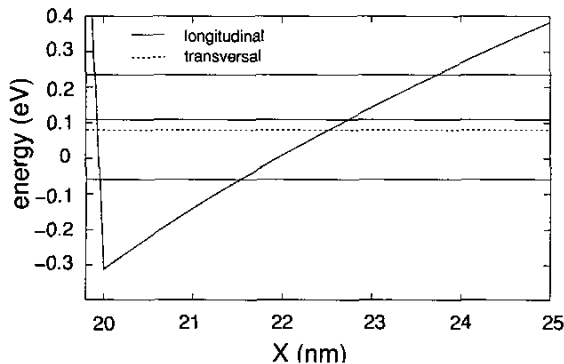

Fig. 3 Conduction band profile and energy of the two-dimensional subbands in mid channel (z = 45 nm) for the bulk Si devices. Solid thin lines indicate subband energy close to the two minima in the conduction band along the kx direction; dotted lines indicate subband energy close to the four minima in the conduction band along the ky and kz directions.

III. RESULTS AND DISCUSSION

The confining potential for electrons in the middle of the channel, for the bulk Si MOSFET, is shown in Fig. 3, along with the subband energies, for $V_{GS} = 1$ V, $V_{DS} = 0.1$ V. In this condition, 96.5% of the total current is carried by the lowest subband.

The output characteristics of the bulk silicon MOSFETs, of the SiGe MOSFET with super-halo doping, and of the SiGe three devices are shown in Figs. 4, 5, and 6, respectively.

The results obtained show that the code is a versatile tool for addressing several different types of devices and materials. It allows us to analyze device performance in a transport regime in which the concept of mobility is not

meaningful. It also allows to tune the threshold voltage and the transconductance by carefully adjusting the layer structure and the doping profiles. Further, extensive simulations and comparison with experimental results are needed to fully validate the code.
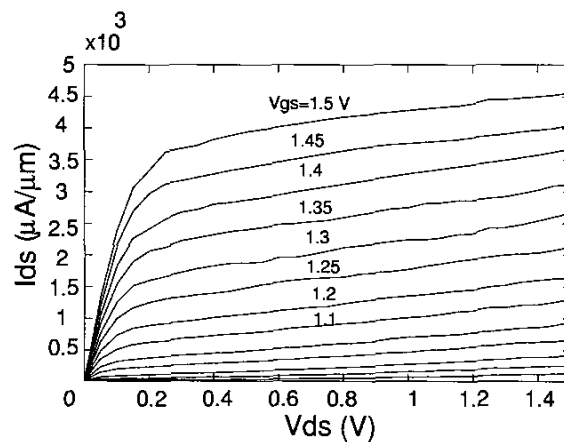
Fig. 4: Output characteristics of the bulk Si 25 nm MOSFET computed with the ballistic current model.
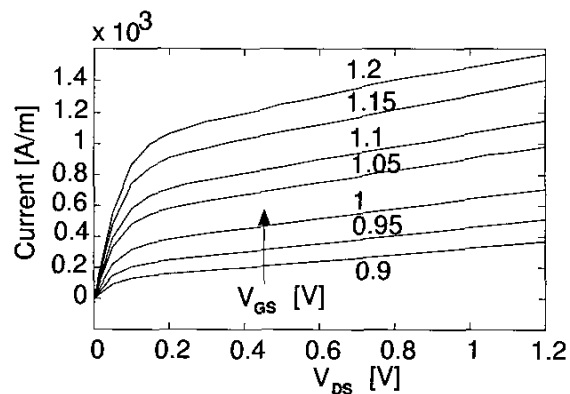

Fig. 5: Output characteristics of the 25 nm strained silicon MOSFET with super-halo p doping shown in Fig. 2.
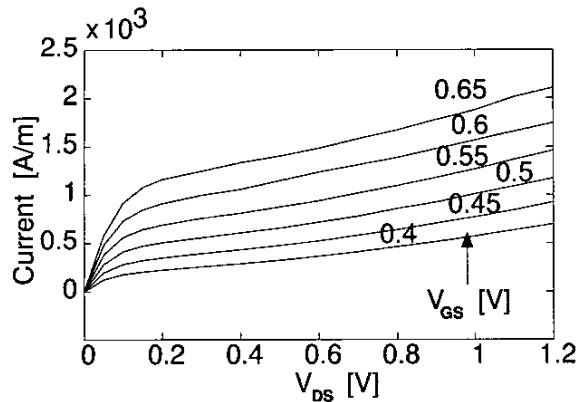
Fig. 6: Output characteristics of the 25 nm strained silicon MOSFET with epitaxial p-doped SiGe layer shown in Fig. 2

REFERENCES

[1] *International Technology Roadmap for Semiconductors*, Semiconductor Industry Association 1999 and 2001.

[2] D. J. Frank, S. E. Laux and M. V. Fischetti, *IEDM Tech. Dig.* pp. 553-556 (1992)

[3] J. D. Bude, "MOSFET Modeling into the nanometer Regime", *SISPAD 2000*, pp. 23-26, 2000.

[4] M. Lundstrom, Z. Ren, S. Datta, *Essential Physics of Carrier Transport in Nanoscale MOSFETs*, SISPAD 2000, pp. 1-5 (2000).

[5] G. Fiori and G. Iannaccone, "The effect of quantum confinement and discrete dopants in nanoscale 50 nm n-MOSFETs: a three-dimensional simulation", *Nanotechnology*, vol. 13 (3), pp. 294-298, 2002.

[6] G. Fiori, G. Iannaccone, submitted to Appl. Phys. Lett., 2002.

[7] G. Curatola and G. Iannaccone, "Quantum confinement in silicon-germanium electron waveguides" *Nanotechnology*, vol. 13(3), pp. 267-273, 2002.

[8] Home page of the well tempered MOSFET at MIT: www.ece.mit.edu/Well