Calibration of the Density-Gradient Model by Using the Multidimensional Effective-Mass Schrödinger Equation

Petru Andrei
ECE Department, Florida State Unviersity and Florida A&M University
Tallahassee, Florida, USA
e-mail: pandrei@eng.fsu.edu

INTRODUCTION

The calibration of phenomenological models of semiconductors is one of the most important tasks in the modeling and analysis of an electronic device. Before a model is used to analyze a semiconductor device, the model parameters should be carefully identified by using more elaborate physical models. In the case of the Density-Gradient model (DGM), the electron and hole effective masses should be computed by using self-consistent Poisson-Schrödinger computations.

The existing methods for the computation of electron and hole effective masses are based on the comparison of the model with 1D Poisson-Schrödinger computations. While this approach is appropriate for devices in which the carriers are confined in only one direction, it is not appropriate for devices in which the carriers are confined in more than one direction, such as short-channel MOSFETs, SOI devices, Fin-FETs, etc. In this article we calibrate the DGM against 2- and 3-dimensional Schrödinger computations. We focus mainly on the computation of electron effective mass, since it enters directly in the equations of the electron current density in n-channel transistors, which are widely used in integrated circuits.

TECHNICAL APPROACH AND DISCUSSION

In the framework of the DGM, the electron concentration at thermal equilibrium can be computed by using the following partial differential equation [1]:

$$\frac{\hbar^2}{12q}\frac{2\nabla\cdot\left(m_{eff,n}^{-1}\nabla\sqrt{n}\right)}{\sqrt{n}}+\varphi-\Phi_n\left(T\right)=0\,, \quad (1)$$

where $\Phi_n\left(T\right)$ is some function that depends on the nature of electron statistics used, $m_{eff,n}$ is the electron effective mass, and all other notations have their usual meaning. Due to the low-order approximations involved in the derivation of (1) it is unrealistic to use the experimental value of $m_{eff,n}$ and the electron effective mass in (1) should be treated as a fitting parameter.

It should be noted that there is no unanimous agreement on the values of $m_{eff,n}$ presented in the literature and the results obtained vary from $0.175m_0$ in [2] to $0.278m_0$ in [3]. The common feature of the existing identification techniques is that $m_{eff,n}$ is calibrated against results obtained by solving the 1D Schrödinger equation in the direction perpendicular to the oxide layer of MOS devices. In this way, it is tacitly assumed that the motion of electrons and holes is quantized only in the direction perpendicular to the oxide and it is described by classical statistics in the other two directions. In the following we present a technique based on the multidimensional effective-mass Schrödinger equation that overcomes the limitations of the existing methods. To simplify numerical computations, let us consider that the electrostatic potential is given a-priori and we can compute the electron concentration by using the effective-mass Schrödinger equation. The electron effective mass can then be computed either by integrating equation (1) or by fitting the electron concentration obtained from (1) to the electron concentration obtained from the Schrödinger equation. This approach has the advantage that it avoids expensive Poisson-

ISBN 3-901578-16-1

Schrödinger computations. Moreover, for particular shapes of the quantum region the eigenvalues and eigenfunctions of the Hamiltonian can be computed analytically and solving the Schrödinger equation numerically can be completely avoided. For example, if we consider a 2D quantum box with infinite walls (see Fig. 1), the electron effective mass depends of the spatial coordinates as in Fig. 2. For a 10×20 nm quantum box in which the electrostatic potential is increasing exponentially, the electron concentration is presented in Fig. 3 for various potential profiles. In these computations $m_{eff,n}$ is assumed constant and it is found by fitting the results obtained by the Schrödinger equation to equation (1).

In Fig. 4 we present the values of the electron effective mass computed for different sizes and shapes of the quantum box. We clearly observe that $m_{eff,n}$ changes from $0.14m_0$ in the case when $L_x \gg L_z$, to $0.24m_0$ for $L_x \ll L_z$. In numerical simulations one should use the value of the electron effective mass which corresponds to the approximate size of the quantum region. In the case of short channel MOSFET devices, $m_{eff,n}$ lies between $0.14m_0$ and $0.24m_0$, depending on the values of W_{eff}/L_{eff} (the effective width divided by the effective length of the conduction channel), as well as on the epitaxial cut of the silicon crystal. For short-channel MOSFET devices, $m_{eff,n}$ is either $0.15m_0$ or $0.24m_0$, depending on whether the x-axis is along or perpendicular to the conduction channel. Our analysis also suggests that the existing discrepancies in the literature on the values of $m_{eff,n}$ originate from the different sizes of the quantum regions used in simulations.

REFERENCES

[1] M. G. Ancona and G. J. Iafrate, *Quantum correction to the equation of state of an electron gas in a semiconductor*, Phys. Rev. B **39**, 9536 (1989).

[2] A. Asenov, S. Slavcheva, A. R. Brown, J. H. Davies, and S. Saini, *Increase in the random dopant induced threshold fluctuations and lowering in sub-100 nm MOSFETs due to quantum effects: A 3-D Density-Gradient simulation study*, IEEE Trans. Electron Devices **48**, 722 (2001).

[3] A. Wettstein, A. Schenk, and W. Fichtner, *Quantum device–simulation using the density–gradient model on unstructured grids*, IEEE Trans. Electron Devices **48**, 279 (2001).

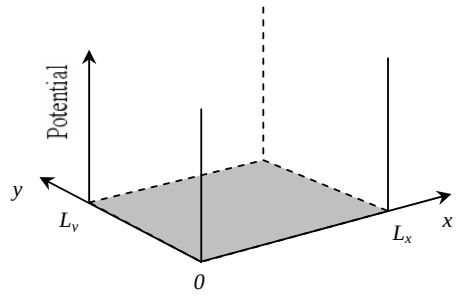

Fig. 1. 2D quantum box with infinite walls.

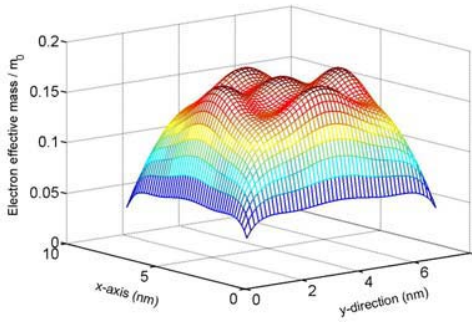

Fig. 2. Electron effective mass computed by integrating eq. (1) , in which *n* was obtained by solving Schrödinger eq. for Si(100).

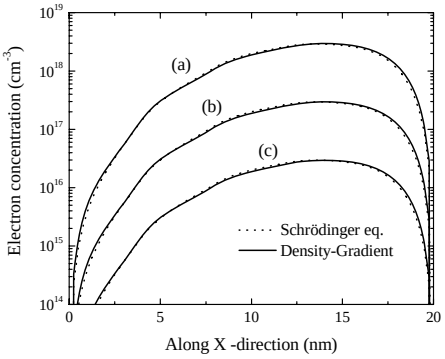

Fig. 3. Electron concentration cross-sections through the middle plane of a 10x20 nm rectangular quantum box.

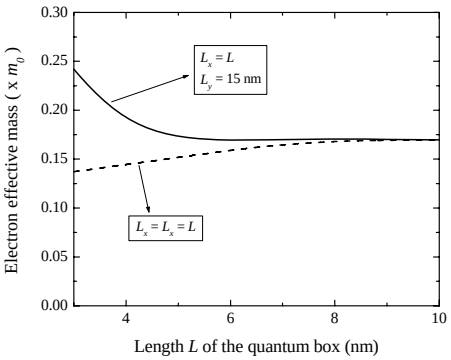

Fig. 4. Electron effective mass that gives the best agreement between the electron concentration computed by using the 2D Schrödinger equation and the 2D Density-Gradient model, respectively, for a rectangular quantum box. The dimensions of the box are indicated on the abscissa.