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Novel Multi-Flux Device Simulation Method Applied to 2DEG Analyses - Drift Diffusion with Subbands -

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Abstract

A novel multi-flux device simulation method proposed by the authors, in which a carrier flux is divided into several carrier fluxes in order to apply different physics model, and to observe the detailed physics in semiconductor devices. In this paper, the multi-flux method is applied to solve 2DEG problems by solving carriers in different subbands independently. Coupled with Poisson-Schrodinger solver, the proposed method enables the detailed modeling of quantum effects of coming novel nano-devices.

1. Introduction

Classical semiconductor device simulation has long been a critical tool to realize new semiconductor devices. Especially the drift-diffusion model is widely used from power devices to edge devices. In order to incorporate quantum effects for nanotechnologies, the density gradient method [1] is also introduced in commercial device simulators. Although the density gradient approach succeeded greatly in modeling nano-devices, the detailed description of the device quantum behavior is not as accurate as the Poisson-Schrodinger approach. The electron quantum confinement creates mixture of the electron distributions of subband carriers, and it is difficult to be described by single quantum potential. These aspects are important in device characteristics, because of the different mobility in each subband arising from 2-fold and 4-fold subbands in a silicon inversion layer for an example.

Recently, the authors have proposed the multi-flux device simulation method in which electrons are divided into several electrons such as electron-1, 2, …, and the method is applied to the modeling of upper valley carriers [2]. In this paper, the method is applied to electrons in subbands of MOSFET inversion layer. Coupled with Poisson-Schrodinger solver, the drift-diffusion model is expanded to analyze detailed distributions of electrons quantumly confined in inversion layers. By the method, electron distributions of different subbands are independently obtained. Thus, the method realizes more detailed modeling of semiconductor devices in nanotechnology era.

2. Simulation method

In conventional device simulation, an electron current continuity equation and a hole current continuity equation are solved self-consistently with Poisson equation for each mesh point. In the proposed multi-flux method, several electron current continuity equations are solved for each mesh point. The simplest set of equations in which two electron continuity equations are solved is shown in Fig. 1. The flux between electron-1 (subband 1) and electron-2 (subband 2) is treated as generation recombination terms. Energy band shifts $\boldsymbol{\Delta E_{C1}}, \boldsymbol{\Delta E_{C2}}, \boldsymbol{\Delta E_{v}}$ are introduced to incorporate quantum effects.

Poisson equation

$$\nabla \cdot (\varepsilon \nabla \psi) = -q(p - n + N_D^+ - N_A^-)$$

Carrier Continuity equation

$$\frac{\partial n_1}{\partial t} = \frac{1}{q}\nabla \cdot \left(-qn_1\mu_{n_1}\nabla(\psi - \Delta E_{C1}) + qD_{n_1}\nabla n_1\right) + GR_{n_1} - GR_{n_{12}}$$

$$\frac{\partial n_2}{\partial t} = \frac{1}{q}\nabla \cdot \left(-qn_2\mu_{n_2}\nabla(\psi - \Delta E_{C2}) + qD_{n_2}\nabla n_2\right) + GR_{n_2} + GR_{n_{12}}$$

$$\frac{\partial p}{\partial t} = -\frac{1}{q}\nabla \cdot \left(-qp\mu_p\nabla(\psi - \Delta E_V) - qD_p\nabla p\right) - GR_{n_1} - GR_{n_2}$$

Fig. 1 An example of minimum set of equations solved in the proposed multi-flux device simulation method. Generation recombination term $\boldsymbol{GR_{n_{12}}}$ governs the flux between electron-1, 2. Energy band shifts $\boldsymbol{\Delta E_{C1}}, \boldsymbol{\Delta E_{C2}}, \boldsymbol{\Delta E_{v}}$ are introduced to incorporate quantum effects.

The simulation method is implemented into Impulse TCAD [3][4] developed using Python programming language. In order to ensure the good numerical convergence, all equations are solved in coupled formalism by Newton-Raphson method. The Jacobian matrix terms are obtained by automatic differentiation library Theano. Thus, Impulse TCAD enables easy implementation of additional equations to device simulation.

Quantum effects are incorporated by energy band shifts obtained by 1D Poisson-Schrodinger method as in [5]. In the proposed method, the first and the second subbands electrons are described by the electron-1 and electron-2. Energy band shifts are those of each electron, and electron distributions are different between the first and the second subbands. Simulation algorithm is schematically shown in Fig. 2.

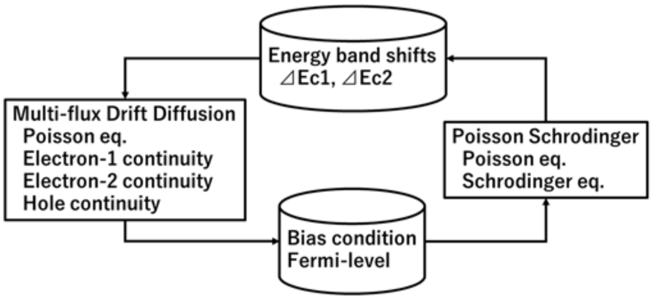

Fig. 2 Algorithm of the proposed method incorporating quantum subband effects.

3. Simulation results

The proposed method is applied to a silicon SOI nMOSFET with effective oxide thickness of 1 nm, SOI thickness of 20 nm, and the channel accepter concentration of 10^{18} /cm^3 as shown in Fig. 3.

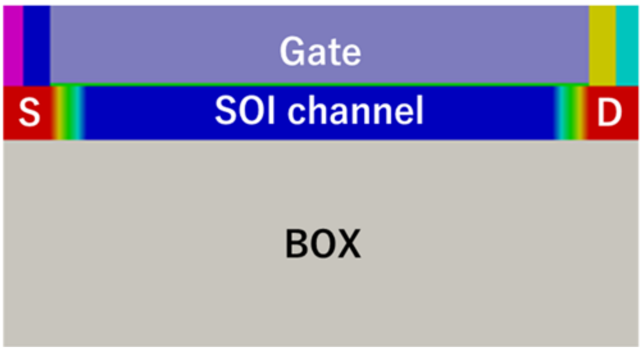

Fig. 3 A silicon SOI nMOSFET used for demonstration of the proposed method.

Poisson-Schrodinger method is applied to vertical 1D MOS capacitor at a few channel lateral positions. Electron Fermi potential is extracted from the drift diffusion device simulation result and is used in Poisson-Schrodinger solver to obtain electron concentrations. Difference of the electron concentration between the Poisson-Schrodinger solver and the drift diffusion device simulation is used to obtain conduction band shifts at each depth point which are feedbacked to the drift diffusion simulation. This changes electron concentration in each subband in the device simulation.

Fig. 4 shows the electron concentration depth profile at the channel center. By the proposed method, the effect of different subbands are incorporated into the multi-fluxes of the drift diffusion method.

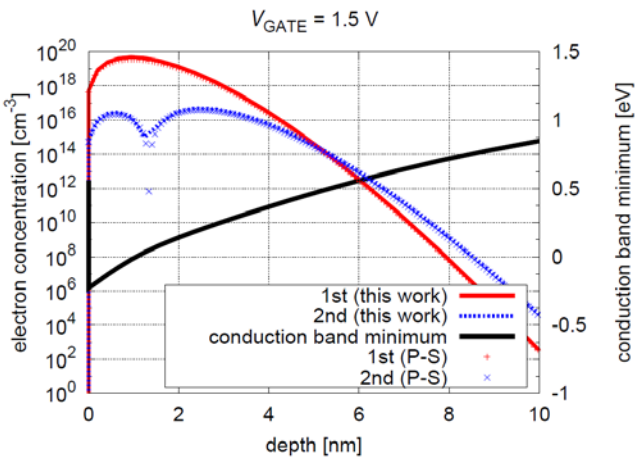

Fig. 4 Electron concentration depth profile at the channel center. The black line shows the conduction band minimum and Poisson-Schrodinger results are shown with markers. The results of the first and the second subbands of the proposed method are shown by the red and the blue line almost identical to Poisson Schrodinger ones.

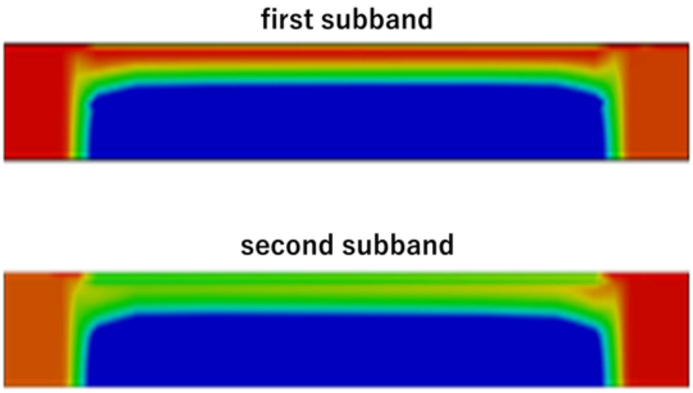

Fig. 5. Two dimensional electron concentration distribution of the first and the second subbands. There are two peaks of concentration along the depth of the second subband electron. Color indicates logarithmic scale of concentration from 10^{10} to 10^{20} cm^{-3}.

Fig. 5 shows the two dimensional electron concentration of the first and the second subbands obtained by the proposed method. The results can be used to describe the different mobility of two-fold and four-fold subbands in a silicon inversion layer.

4. Conclusions

The multi-flux device simulation method is applied to the 2DEG problem. In the demonstration, the first and the second subband electrons are treated as two electron fluxes. Coupled with Poisson-Schrodinger solver, the simple drift diffusion simulator is expanded to incorporate quantum effects. It is worth mentioning that this approach enables detailed modeling of nano-devices, such as carrier mobility depending of the subbands, for an example..

References

[1] Ancona, M. G., Yu, Z., Dutton, R. W., Voorde, P. V., Cao, M., and Vook, D. (2000). Density-gradient analysis of MOS tunneling. IEEE transactions on Electron Devices, 47(12), 2310-2319.

[2] K. Fukuda *et al, EDISON21, 2019.*

[3] T. Ikegami, K. Fukuda, J. Hattori, H. Asai, and H. Ota, J. Comp. Electron., 1-9 (2019)

[4] https://unit.aist.go.jp/neri/en/ImpulseTCAD/index.html

[5] Huang, C. K., & Goldsman, N. (2001). 2-D self-consistent solution of Schrödinger equation, Boltzmann transport equation, Poisson and current-continuity equation for MOSFET. SISPAD 2001, 148-51.