Modelling Quantum Transport in Nanostructures

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Abstract: *In recent years the state of art semiconductor technology has motivated engineers across the globe to design devices having dimensions in nanoscale regime. At this scale minima, the transport within the device is dominated by quantum mechanics. This paper reviews threeimportant variants of Non-equilibrium Green's Function (NEGF) used for modellingquantum transport within nanostructures.*

I. Introduction:

Basic quantum transport mechanism can be classified as (i) dissipative transport (ii) ballistic transport ($L_{device} \approx \lambda_{free}$) and (iii) tunneling transport ($L_{device} << \lambda_{free}$).

Number of methods have been suggested in past decade to explain the quantum transport mechanism. Among the most commonly used formulizing schemes are the Wigner-function approach, the Pauli master equation, and the non-equilibrium Green's functions (NEGF).In order to study the extremely scaled MOSFET devices it is essential to know quantum transport modelling so as to address design issues and electrical characterization. Three basic methods of quantum transport namely Non equilibrium Green's function formalism, recursive Green's function algorithm and Gu method are compared in this review work based on Mat lab simulations of these formalism.[1-8]

II. Non-equilibrium Green Function: Traditional Method

The non-equilibrium Green's function formalism (NEGF) provides a rigorous description of quantum transport in nanoscale devices. The method is composed of two main blocks, Poisson's equation solver and the quantum transport solver which is based on the NEGF formalism. Poisson's equation gives the electrostatic potential distribution (V) with in the nano structure for a given electron density (n) and hole density (p). The NEGF solver gives the n and p density and the electrical current (I) for an applied potential V. The self-consistent method starts by assuming initial value for the potential which is fed to the NEGF solver to calculate the n and p densities. The calculated densities are fed to Poisson's solver to find the updated potential V in the nano-structure. The equations are solved using looping construct between Poisson's solver and NEGF solver until the update in the potential drops below certain tolerance, after which the terminal currents are estimated. The device geometry of the double gate MOSFET under consideration is shown in the figure 1 .Following assumptions have been made during simulation [3-8][11-20]
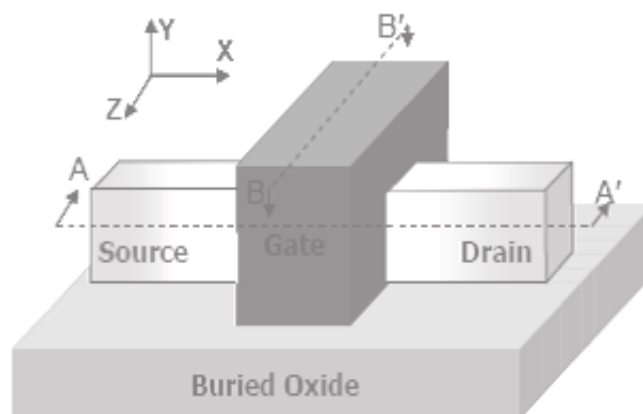

Figure-1

(1) height ('Y'-Coordinate) of the Fin FET is much larger compared to the width (Z- coordinate) (Figure 1) so that it is reasonable to assume that carriers are not confined along Y direction and solution of the Schrodinger Equation can be represented by simple plane waves and,

(2) the device can be viewed as a combination of parallel identical slices along the Y direction.

(3) The metal contacts are so large such that thermal equilibrium is maintained and the Fermi level in these regions is determined by the applied voltage.

(4) N-channel transistor where holes contribution, to both the transport and the electrostatic problems, can be neglected.

(5) No electron penetration in the insulator region.[2][4]

A single band effective mass Hamiltonian [16] is used to model the electron transport. The 2D wave function $\psi(x, y)$ is obtained from the solution of the 2D Schrödinger equation:

$$\left[-\frac{\hbar^2}{2} \left(\frac{1}{m^*_x{}^2} \frac{\partial^2}{\partial_x^2} + \frac{1}{m^*_y{}^2} \frac{\partial^2}{\partial_y^2} \right) + E_C(x, y) \right] \Psi(x, y) = E_l \Psi(x, y) \qquad \text{--------------------} \quad (1)$$

Where m^*_x and m^*_y =electron effective mass in x and y-direction respectively. Ec is the conduction band edge and El is the longitudinal energy due to motion in x- and y-direction respectively.[5]

The equation representation using Hamiltonian matrix is

$$[H_l]\{\psi\} + [E_C]\{\psi\} = [E_l I]\{\psi\} \qquad \text{-----------------------------}$$
$$(2)$$

Where each of these terms in matrix form are as

$$H_l = \begin{bmatrix} \alpha & \beta & O...... & .O \\ \beta & \alpha & \beta...... & O \\ O & ... & .... & .... \\ ... & ... & .... & \beta\alpha \end{bmatrix}_{NxNy*NxNy} \qquad \alpha = \begin{bmatrix} 2t_x + 2t_y & -t_y & 0...... & .0 \\ -t_y & 2t_x + 2t_y & ...... & 0 \\ 0 & ... & .... & .... \\ ... & ... & .... & -t_y 2t_x + 2t_y \end{bmatrix}_{Ny*Ny}$$

$$\beta = \begin{bmatrix} -t_x & 0 & 0...... & .0 \\ 0 & -t_x & ...... & 0 \\ 0 & ... & .... & .... \\ ... & ... & .... & -t_x \end{bmatrix}_{Ny*Ny} \qquad E_C = \begin{bmatrix} E_{C1} & 0 & 0...... & .0 \\ 0 & E_{C2} & ...... & 0 \\ 0 & ... & .... & .... \\ ... & ... & .... & E_{CN_xN_y} \end{bmatrix}_{N_xNy*N_xNy} \qquad \Psi = \begin{bmatrix} \Psi_1 \\ \Psi_2 \\ . \\ \psi_{NxNy} \end{bmatrix}_{N_xNy*1}$$

$$t_x = \frac{\hbar^2}{2m^* *(\Delta x)^2} \text{ and } t_y = \frac{\hbar^2}{2m^*_y (\Delta y)^2}$$

Using self-energy concept within NEGF framework and considering only active area within the device with boundary conditions and including source and drain self- energy expressions as $\sum_{source}$ and $\sum_{Drain}$ respectively;Non-equilibrium Green equation for an active device is written as

$$G = \frac{1}{[E_l I - (H_l + E_C) - \sum_{source} - \sum_{Drain}]} \qquad \text{------------------------------------} \quad (3)$$

Values of $\sum_{source}$ and $\sum_{Drain}$ are

$$\sum Source = \begin{bmatrix} \beta g_s \beta & 0 & 0 & 0 \\ & .. & .. & \\ & & .. & \\ 0 & .. & & 0 \end{bmatrix}_{NxNyXNxNy} \qquad \sum Drain = \begin{bmatrix} 0 & 0 & 0 & 0 \\ & .. & .. & \\ & & .. & \\ 0 & .. & & \beta g_D \beta \end{bmatrix}_{NxNyXNxNy} \qquad \text{------------} \quad (4)$$

Where g_s and g_D are surface Green's functions of the source and drain contacts respectively. The carrier transport is represented by the broadening function at source and drain terminals representing

$$\Gamma_S = i\left[\sum S - \sum{}_S^+\right] \text{and} \Gamma_D = i\left[\sum D - \sum{}_D^+\right] \qquad \text{-------------------------------------(5)}$$

By considering spectral function ,quantum transport phenomena representation at source and drain terminals can be summed a

$$A_S = G\Gamma_S G^+ \text{ and } A_D = G\Gamma_D G^+ \qquad \text{--------------------------(6)}$$

Considering Fermi equation, Fermi levels of source and drain are evaluated with correlation function

$$G^n(E_l) = A_S(E)F(E_l, E_{fS}) + A_D(E)F(E_l, E_{fD}) \qquad \text{----------------------------------} \quad (7)$$

The transmission coefficient from the source contact terminal to drain contact is defined in terms of Green's function and broadening function as

$$T_{SD} = Trace\left[\Gamma_S G\Gamma_D G^+\right]\text{----------------------------------(8)}$$

Total electron density and current are estimated by integrating over longitudinal energy E_l and summing over all the conduction band valleys.

Numerical matrix inversion consumes a large number of operations that in the order of N_{grid}^3. Green's function is calculated for each energy point considered in the simulation. This makes total number of operations on the scale of $N_{operations} = N_{Energypoints} N_{grid}^3$. [4-8]

III.   The Recursive Green function:

The computational efforts can easily be minimized by considering device 2D symmetry and computing Green function recursively without full inversion of Hamiltonian matrix. It can be used only if the effective Hamiltonian matrix is block tri-diagonal. As the nano device has only two contacts and there exists coupling between nearest neighboring layers; recursive Green function logic is applicable and yields good results without compromising the accuracy. The equations under consideration can be summarized as

$D = [E_l I - H_d - \sum_S - \sum_D]$ dimension $D_{n,m}$ denotes $D[(n-1)N_y : nN_y, (m-1)N_y : mN_y]$ from which Non equilibrium Green function is computed using following steps:

a) $g_{1,1}^{L1} = D_{1,1}^{-1}$

b)   For   q=1,2,3… N_X-1,Values   of   g   are   computed   as
$g_{q+1,q+1}^{Lq+1} = \left(D_{q+1,q+1} + D_{q+1,q} g_{q,q}^{Lq} D_{q,q+1}\right)^{-1}$ and also $g_{q,q}^{+Lq}$

c) $G_{Nx,Nx} = g_{Nx,Nx}^{LNx}$

d)   For q values N_X-1 …..,1 Compute all the values as; $G_{q,q+1} = \left(- g_{q,q}^{Lq} D_{q,q+1} G_{q+1,q+1}\right);$

$g_{q+1,q} = \left(G_{q+1,q+1} D_{q,+1,q} g_{q,q}^{Lq}\right)$-- for $G_{q,q+1}^+$ and $G_{q+1,q}^+$

Assuming only source and drain contacts to be conducting

$\sum^{in}(E_l) = \Gamma_S(E_l)F(E_l, E_{fs}) + \Gamma_S(E_l)F(E_l, E_{fD})$ the Green function value is calculated for q= 1,2,..N_X-1 using steps as

a) $\quad g_{1,1}^{nL1} = g_{1,1}^{L1} \sum_{11}^{L1} \sum_{11}^{in} g_{1,1}^{L1^+}, \quad$ and $g_{q+1,q+1}^{nLq+1} = g_{q+1,q+1}^{Lq+1}\left[\sum_{q+1,q}^{in} + D_{q+1,q}g_{q,q}^{nLq}D_{q,q+1}^+\right]g_{q+1,q+1}^{Lq+1^+}$

and for q=1,2…. N_X-1

b) $\quad G_{Nx,Nx}^n = g_{Nx,Nx}^{nLNx}$ ….

c) $\quad$ Computing

$G_{q,q}^n = g_{q,q}^{nLq} + g_{q,q}^{Lq}\left(D_{q,q+1}G_{q+1,q+1}^n D_{q+1,q}^+\right)g_{q,q}^{+Lq} - \left[g_{q,q}^{Lq}D_{q,q+1}^+ G_{q+1,q}^+ + G_{q,q+1}D_{q+1,q}g_{q,q}^{nLq}\right]_{\text{For}}$

q= N_X-1,N_X-2……1 $\quad$ and then apply $G_{q,q+1}^n = G_{q+1,q}^{+n}$ The longitudinal energy resolved electron density at a grid point I is estimated form diagonal elements .The y direction computation is based on inverse Hamiltonian matrix and N_x values correspond to inversion of each vertical energy layer. The total number of steps in the computation are thus $N_{operations} = N_{Energypoints}N_y^3 N_x$ [3-8][10]

IV.   The Gauss Estimation Method:

The method does not consider the entire Green's function, but computes spectral coefficients for representation based on sparse nature of broadening function. The Non-equilibrium Green's function carrier transport at drain and source contacts can be expressed in matrix form as

$$\Gamma_S = \begin{bmatrix} [\beta(g_S - g_S^+)\beta]_{NyXNy} & 0 & 0 & 0 \\ & 0 & 0 & 0 \\ & & & \\ 0 & & 0 & 0 \end{bmatrix}_{NxN_yXNxN_y} \quad \Gamma_D = \begin{bmatrix} 0 & 0 & 0 & 0 \\ & 0 & 0 & 0 \\ & & & \\ 0 & 0 & [\beta(g_D - g_D^+)\beta]_{NyXNy} \end{bmatrix}_{NxN_yXNxN_y}$$

Rather than computing current by integrating over entire longitudinal field it is computed for discrete values by Green's function as

$G_S = [E_l I - H_l - \Sigma_S - \Sigma_D]/I_S$ and $G_D = [E_l I - H_l - \Sigma_S - \Sigma_D]/I_D$ ----------- (9)

Due to consideration of discrete values only $N_x N_y X 2N_y$ are considered. The final transport equation is [3][5][7][8][10][18-20]

$$T_{SD} = Trace\left(\left[\beta(g_s - g_S^+)\beta\right]G_{DS}\left[\beta(g_D - g_D^+)\beta\right]G_{DS}^+\right)$$

Where $G_{DS} = \begin{bmatrix} G(1,(Nx-1)Ny+1) & G(1,(Nx-1)Ny+2) & .... & G(1,Ny) \\ & & & \\ & & & \\ G(Ny,(Nx-1)Ny+1) & & & G(Ny,Ny) \end{bmatrix}_{NyXNy}$

V.   Conclusion:

All the three simulation techniques are simulated using Mat lab In each of the concepts applied the number of iterations as well as number of terms get reduced. The approximations made due to submicron structural dimensions help to yield results faster without compromising accuracy.

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