11

Master Equation - Based Numerical Simulation in a Single Electron Transistor Using Matlab

Ratno Nuryadi
Center for Material Technology
Agency for Assessment and Application of Technology, Jakarta
Indonesia

1. Introduction

Recent modern fabrication technology allows us for the fabrication of nanometer-scaled devices, which is possible to observe single electronic or single electron tunneling phenomena (Averin & Likharev, 1991; Likharev, 1988; Likharev, 1999; Hanna et al., 1991; Tucker, 1992). On the other hand, MOSFET (metal-oxide-semiconductor field effect transistor) devices with channel length below 20 nanometer (nm) are no more properly operated because the down-scaling of MOS devices causes a large statistical fluctuation of the threshold voltage. A possible approach to overcome this problem is to use the single electron devices for future VLSI (very large scale integrated circuit) (Takahashi et al., 1995; Saitoh et al., 2001).
Nanometer scale single electron devices have the following features, i.e., low power consumption and small size. These are key features to realize ultra high density circuits. Single electron circuits with new architecture are also possible because the basic operation of single electron devices is quite different from that of conventional semiconductor devices.
There are two major requirements for single electron tunneling phenomena (Coulomb blockade) to occur (Averin & Lhikarev, 1991; Likharev, 1988; Likharev, 1999). Firstly, thermal energy $k_B T$ must be much smaller than elemental charging energy $e^2/2C$. This ensures that the transport of charges is in fact governed by the Coulomb charging energy. This condition can be fulfilled either by lowering the temperature or by decreasing the capacitance which means to reduce the island size. Usually, experiments are performed at temperatures of a few mK and for structures with island sizes of a few hundred nanometers. Second requirement is related to tunnel resistance which must exceed the quantum resistance ($h/4e^2 \approx 6.5$ kΩ). This condition ensures that the wave functions of excess electrons between the barriers are basically localized. On the other word, in the case of lower tunnel resistance, excess charges extend over the barriers so that no single electron tunneling event can be possible.
There are several types of circuits where the single electron tunneling phenomena are being explored, such as single electron box (Likharev, 1999), single electron transistor (SET) (Tucker, 1992; Takahashi et al., 1995; Saitoh et al., 2001; Wolf et al., 2010; Sun et al., 2011; Lee et al., 2009), single electron pump (Ono et al., 2003), single electron turnstile (Moraru et al., 2011) and single electron circuits with several junctions (1D and 2D arrays) (Nuryadi et al., 2003; Nuryadi et al., 2005). A double junction system is most important single electron circuit because of a basic component of SET. At small applied voltage, the system remains in the Coulomb blockade state, and no current flows through the double junctions. On the other hand, at higher applied

voltage, the Coulomb blockade is defeated and the electrons can tunnel through the junctions and finally the current flows. If the island between two tunnel junctions is electrostatically controlled by the gate capacitance, the system became single electron transistor. This device is reminiscent of a MOSFET, but with a small island (dot) embedded between two tunnel capacitors/junctions, instead of the usual inversion channel.

It is well known that a numerical simulation of the devices could help a great deal in their understanding of the devices. However, although so far several groups have reported the simulation and modeling of single electron tunneling devices (Amman et al., 1991; Kirihara et al., 1994; Fonseca et al., 1997; Wasshuber et al., 1997; Nuryadi et al., 2010), numerical simulation with detail explanation and easy examples is still needed, especially for beginners in the field of single electron devices. Basically there are two methods to simulate the single electron phenomena, i.e., master equation (Amman et al., 1991; Nuryadi et al., 2010) and Monte Carlo methods (Kirihara et al., 1994; Fonseca et al., 1997; Wasshuber et al., 1997).

The goal of this chapter is to simulate numerically current-voltage characteristics in the single electron transistor based on master equation. A master equation for the probability distribution of electrons in the SET dot (see Fig. 1) is obtained from the stochastic process, allowing the calculation of device characteristics. First, I will start with an introduction of the basic equations in Master equation (section II). Next, the derivation of free energy change due to electron tunneling event is discussed in section III. The flowchart of numerical simulation based on Master equation and the Matlab implementation will be discussed in section IV and V, respectively. The examples of simulation resuls are presented in section V. Finally, section VI is conclusion.

2. Basic equations in master equation based simulation

Figure 1 shows the SET circuit consisting of a dot between the source and drain electrodes separated by tunnel capacitors C_1 and C_2. Both tunnel capacitors C_1 and C_2 have tunnel resistances R_1 and R_2, respectively. The dot is also coupled to the gate electrode with capacitor C_G in order to control the current flow. The total capacitance between the dot and the outer environment can be writen as C_Σ, where

$$C_\Sigma = C_1 + C_2 + C_G. \tag{1}$$

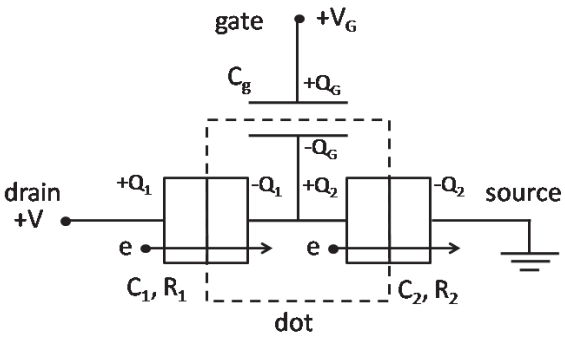


Fig. 1. Single electron transistor has a structure of the dot in the center coupled by two tunnel capacitors (C_1 and C_2) and a gate capacitor C_G. Source is connected to a ground, where drain and gate are applied by voltages V and V_G (Tucker, 1992).

There are four main equations for current-voltage characteristics of single electron circuits, i.e., free energy change ΔF, tunneling probability/rate Γ, steady state master equation and current equation I, as follows.

Free energy change:

$$\Delta F_1^{\pm}(n_1, n_2) = \frac{e}{C_\Sigma}\left\{\frac{e}{2} \pm (Ne - Q_0) \mp (C_G + C_2)V \pm C_G V_G\right\} \tag{2a}$$

$$\Delta F_2^{\pm}(n_1, n_2) = \frac{e}{C_\Sigma}\left\{\frac{e}{2} \mp (Ne - Q_0) \mp C_1 V \mp C_G V_G\right\} \tag{2b}$$

Tunneling probability/rate:

$$\Gamma_1^{\pm}(N) = \frac{1}{R_1 e^2}\left[\frac{-\Delta F_1^{\pm}}{1 - exp\left[\Delta F_1^{\pm}/k_B T\right]}\right] \tag{3a}$$

$$\Gamma_2^{\pm}(N) = \frac{1}{R_j e^2}\left[\frac{-\Delta F_2^{\pm}}{1 - exp\left[\Delta F_2^{\pm}/k_B T\right]}\right] \tag{3b}$$

Steady State Master equation:

$$\rho(N)[\Gamma_2^{-}(N) + \Gamma_1^{+}(N)] = \rho(N+1)[\Gamma_2^{+}(N+1) + \Gamma_1^{-}(N+1)] \tag{4}$$

Current equation:

$$I(V) = e\sum_{N=-\infty}^{\infty}\rho(N)[\Gamma_1^{+}(N) - \Gamma_1^{-}(N)] = e\sum_{N=-\infty}^{\infty}\rho(N)[\Gamma_2^{+}(N) - \Gamma_2^{-}(N)] \tag{5}$$

where e is the elemental charge, k_B is the Boltzmann constant, T is the temperature, N is the number of electrons in the dot, n_1 and n_1 are a number of electrons flows through the capacitor C_1 and capacitor C_2, respectively, Q_0 is the background charge and +/- express that the electron tunnels through the capacitor with the direction from left to the right and from right to the left, respectively.

Equations (2a) and (2b) are used to calculate the free (electrostatic) energy change ΔF of the system due to the one electron tunneling event. It is important to be noted that only tunneling events decreasing the electrostatic energy (and dissipating the difference) are possible.

The values ΔF from equations (2a) and (2b) are used to calculate electron tunneling probability in the equations (3a) and (3b), respectively. The tunneling of a single electron through a particular tunnel junction is always a random event, with a certain rate Γ (i.e., probability per unit time) which depends solely on the ΔF. Equation (4) expresses the Master equation in steady state, resulting the value of $\rho(N)$, which is necessary to be used for the current calculation in equation (5).

3. Derivation of free energy change in single electron transistor circuit

As explained above that the free energy change of the system before and after tunnel event plays a key role on the occurrence of the electron tunneling, i.e., whether the tunneling event occurs or dot. Therefore, the origin of the free energy change in SET system is important to be reviewed. The free energy of voltage-biased single electron transistor is defined by the difference in electrostatic energy stored in the circuit (total charging energy) and work done by the external voltage source due to tunnel events.

3.1 Total charging energy

In order to calculate total charging energy, it is necessary to determine the voltage applied on the tunnel capacitor C_1 (V_1) and tunnel capacitor C_2 (V_2) using the following step. The configuration of the charges on each capacitor in the single-electron transistor circuit (Figure1) can be expressed as (Tucker, 1992),

$$Q_1 = C_1V_1 = C_1(V - V_2), \tag{6a}$$

$$Q_2 = C_2V_2, \tag{6b}$$

$$Q_G = C_G(V_G - V_2). \tag{6c}$$

It is noted that the V_2 is also subjected to the voltage in the dot. Charge in the dot is given by,

$$Q = Q_2 - Q_1 - Q_G = Ne - Q_0. \tag{7}$$

Here, $N = n_1 - n_2$ is a number of electrons in the dot.
If the equations (6a), (6b) and (6c) are inserted into an equation (7), it can be obtained the V_2 as a function of drain voltage V and gate voltage V_G, as follows,

$$C_2V_2 - C_1(V - V_2) - C_G(V_G - V_2) = Q,$$

$$V_2 = \frac{1}{C_\Sigma}(C_1V + C_GV_G + Q) \tag{8}$$

From equation (8) and relationship of $V_1 + V_2 = V$, it can be obtained the value of voltage on capacitor C_1, as follows,

$$V_1 = V - \frac{1}{C_\Sigma}(C_1V + C_GV_G + Q)$$

$$V_1 = \frac{1}{C_\Sigma}[(C_2 + C_G)V - C_GV_G - Q] \tag{9}$$

Note that both V_1 and V_2 are a function of N, which is the number of electrons in the dot because of $Q = Ne - Q_0$.
Next, total charging energy on the SET system can be calculated as follows,

$$E_c = \frac{Q_1^2}{2C_1} + \frac{Q_2^2}{2C_2} + \frac{Q_G^2}{2C_G}$$

$$E_c = \frac{1}{2C_\Sigma}[C_GC_1(V - V_G)^2 + C_1C_2V^2 + C_GC_2V_G^2 + Q^2] \tag{10}$$

Since the values of external power supply V and V_G is constant, the effect on electron tunneling process only influences the term of $Q^2/2C_\Sigma$.

3.2 Work done by external voltage source due to tunnel event

There are two types of tunnel events, i.e., electron tunnels through the capacitor C_1 and the electron tunnels through the capacitor C_2. The amount of the work done by external voltage source is different from one event to another one. Therefore, the detail explanation of the work done for these two types is discussed. Figure 3 shows the charge flow enter/exit from the voltage source when the electron tunnel through the capacitor C_1 (right direction).

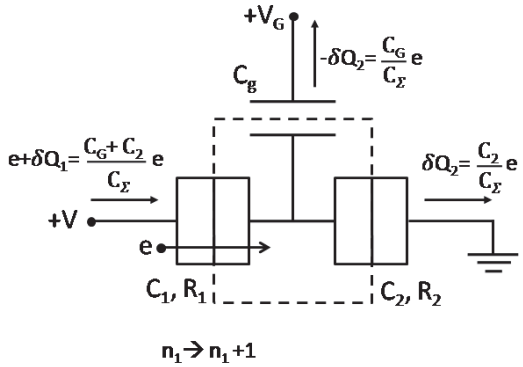


Fig. 3. The charge flow in the single electron transistor circuit when one electron through the capacitor C_1 (Tucker, 1992).

Work done by the power supply when the electron tunnel through the capacitor $C_1$is formulated as follows:

1. Change in charge when one electron tunnels through capacitor $\boldsymbol{C_1}$ $(\boldsymbol{n_1 \longrightarrow n_1 + 1})$

Change of dot potential due to this electron tunneling $(Q \longrightarrow Q + e$ or $N \longrightarrow N + 1)$ is $\delta V_2 = V_2^{after} - V_2^{before}$, thus:

$$\delta V_2 = \frac{1}{C_\Sigma}\left(C_1 V + C_G V_G + (Q + e)\right) - \left[\frac{1}{C_\Sigma}(C_1 V + C_G V_G + Q)\right]$$

$$\delta V_2 = \frac{e}{C_\Sigma} \tag{11}$$

It is noted that V_2^{after} and V_2^{before} express the values of V_2 after and before tunneling, respectively.

Change of charge in capacitor C_1 is $\delta Q_1 + e$, where $\delta Q_1 = Q_1^{after} - Q_1^{before}$. Consider the equation (6a) it is obtained the below relationship,

$$\delta Q_1 = C_1\left(V - V_2^{after}\right) - C_1\left(V - V_2^{before}\right),$$

$$\delta Q_1 = -C_1 \delta V_2. \tag{12}$$

By inserting equation (11) into equation (12), it is obtained

$$\delta Q_1 = -\frac{C_1}{C_\Sigma}\mathrm{e}$$

Therefore, total change of the charge in capacitor C_1 is,

$$\delta Q_1 + e = -\frac{C_1}{C_\Sigma}\mathrm{e} + \mathrm{e}$$

$$\delta Q_1 + e = \frac{C_2 + C_G}{C_\Sigma} e \tag{13}$$

Change of charge in capacitor C_2 is $\delta Q_2 = Q_2^{after} - Q_2^{before}$. Consider the equation (6b) δQ_2 becomes,

$$\delta Q_2 = C_2 V_2^{after} - C_2 V_2^{before},$$

$$\delta Q_2 = C_2 \delta V_2,$$

$$\delta Q_2 = \frac{C_2}{C_\Sigma} \mathrm{e} \tag{14}$$

Change of charge in capacitor C_G is $\delta Q_G = Q_G^{after} - Q_G^{before}$. Consider the equation (6c) δQ_G becomes,

$$\delta Q_G = C_G\left(V_G - V_2^{after}\right) - C_G\left(V_G - V_2^{before}\right),$$

$$\delta Q_G = -C_G \delta V_2,$$

$$\delta Q_G = -\frac{C_G}{C_\Sigma} \mathrm{e} \tag{15}$$

2. Work done when one electron tunnel through capacitor $\boldsymbol{C_1}$ $(\boldsymbol{n_1 \longrightarrow n_1 + 1})$

Work done by power supply is a sum of multiplication between charge change in each terminal and a given power supply voltage. Thus, when one electron tunnel through the capacitor C_1, the work becomes,

$$W_S(n_1) = n_1[(e + \delta Q_1)V + (\delta Q_G)V_G + (\delta Q_2) \times 0],$$

$$W_S(n_1) = n_1\left[\frac{C_G + C_2}{C_\Sigma} eV - \frac{C_G}{C_\Sigma} eV_G\right] \tag{16}$$

The same calculation can be done when the single electron tunnel through the capacitor C_2, as shown in Figure 3.

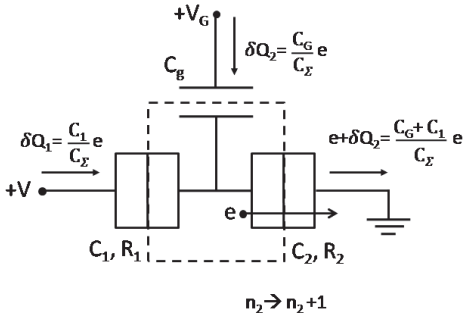


Fig. 3. The charge flow in the single electron transistor circuit when an electron tunnels through the capacitor C_2.

1. Change in charge when an electron through the capacitor $\boldsymbol{C_2}$ $\boldsymbol{(n_2 \longrightarrow n_2 + 1)}$

Change of potential in the dot due to electron tunneling $(Q \longrightarrow Q - e$ or $N \longrightarrow N - 1)$ is $\delta V_2 = V_2^{after} - V_2^{before}$, thus :

$$\delta V_2 = \frac{1}{C_\Sigma}(C_1 V + C_G V_G + (Q - e)) - \left[\frac{1}{C_\Sigma}(C_1 V + C_G V_G + Q)\right],$$

$$\delta V_2 = -\frac{e}{C_\Sigma} \tag{17}$$

Change in charge on a capacitor C_1 is $\delta Q_1 = Q_1^{after} - Q_1^{before}$. Consider the equation (6a), δQ_1becomes,

$$\delta Q_1 = C_1\left(V - V_2^{after}\right) - C_1\left(V - V_2^{before}\right),$$

$$\delta Q_1 = -C_1 \delta V_2,$$

$$\delta Q_1 = \frac{C_1}{C_\Sigma}\mathrm{e} \tag{18}$$

Change in the charge on a capacitor C_2 is $\delta Q_2 + e$, where $\delta Q_2 = Q_2^{after} - Q_2^{before}$. Consider the equation (6b), δQ_2becomes,

$$\delta Q_2 = C_2 V_2^{after} - C_2 V_2^{before},$$

$$\delta Q_2 = C_2(\delta V_2),$$

$$\delta Q_2 = -\frac{C_2}{C_\Sigma}\mathrm{e}$$

So the total change in charge on the capacitor C_2 is,

$$\delta Q_2 + e = -\frac{C_2}{C_\Sigma}\mathrm{e} + \mathrm{e},$$

$$\delta Q_2 + e = \frac{C_1 + C_G}{C_\Sigma} e \tag{19}$$

Changes in the charge on a capacitor C_G is $\delta Q_G = Q_G^{after} - Q_G^{before}$. Consider equation (6c), δQ_G becomes,

$$\delta Q_G = C_G\left(V_G - V_2^{after}\right) - C_G\left(V_G - V_2^{before}\right),$$

$$\delta Q_G = -C_G \delta V_2,$$

$$\delta Q_G = \frac{C_G}{C_\Sigma}\mathrm{e} \tag{20}$$

2. Work done when one electron through the capacitor $\boldsymbol{C_2}$ $(\boldsymbol{n_2 \longrightarrow n_2 + 1})$

From the above calculation, the work done by the power supply when the electrons tunnels through the capacitor C_2 becomes

$$W_S(n_2) = n_2[(\delta Q_1)V + (\delta Q_G)V_G + (e + \delta Q_2) \times 0],$$

$$W_S(n_2) = n_2\left[\frac{C_1}{C_\Sigma} eV + \frac{C_G}{C_\Sigma} eV_G\right] \tag{21}$$

3.3 Free energy

The most important requirement for the accurence of single electron tunneling is that the total energy of the transistor system must decrease due to one electron tunneling. In the other word, the electron tunneling will not occur if the total energy of the system increases due to the electron tunneling. This condition is called as Coulomb blockade. The free energy is defined by the difference in the total charging energy and total work done by the power supply, as follows:

$$F(n_1, n_2) = E_c - W_S^{total},$$

$$F(n_1, n_2) = \frac{Q^2}{2C_\Sigma} - \left\{ n_1 e \left[\frac{C_G + C_2}{C_\Sigma} V - \frac{C_G}{C_\Sigma} V_G \right] + n_2 e \left[\frac{C_1}{C_\Sigma} V + \frac{C_G}{C_\Sigma} V_G \right] \right\} + constant \tag{22}$$

3.4 Change in free energy due to tunnel event

Change in free energy after and before electron tunneling will determine whether the electron tunneling occurs or not. If the system becomes more stable (energy decreases) when the electron tunnels, electron tunneling will occur. Let's look at the conditions when the electron tunnels through the capacitor C_1. The free energy change after and before tunneling can be calculated as follows:

$$\Delta F_1^{\pm}(n_1, n_2) = F(n_1 \pm 1, n_2) - F(n_1, n_2),$$

$$\Delta F_1^{\pm}(n_1, n_2) = \left\{ \frac{(Q \pm e)^2}{2C_\Sigma} - \left\{ (n_1 \pm 1) e \left[\frac{C_G + C_2}{C_\Sigma} V - \frac{C_G}{C_\Sigma} V_G \right] + n_2 e \left[\frac{C_1}{C_\Sigma} V + \frac{C_G}{C_\Sigma} V_G \right] \right\} \right\} - \left\{ \frac{Q^2}{2C_\Sigma} - \left\{ n_1 e \left[\frac{C_G + C_2}{C_\Sigma} V - \frac{C_G}{C_\Sigma} V_G \right] + n_2 e \left[\frac{C_1}{C_\Sigma} V + \frac{C_G}{C_\Sigma} V_G \right] \right\} \right\}$$

$$\Delta F_1^{\pm}(n_1, n_2) = \frac{e}{C_\Sigma} \left\{ \frac{e}{2} \pm Q \mp (C_G + C_2) V \pm C_G V_G \right\} \tag{23}$$

By inserting $Q = Ne - Q_0$ into equation (23), the equation (2a) is obtained.

On the other hand, when the electron tunnels through the capacitor C_2, the free energy change when the after and before tunneling is calculated as follows:

$$\Delta F_2^{\pm}(n_1, n_2) = F(n_1, n_2 \pm 1) - F(n_1, n_2),$$

$$\Delta F_2^{\pm}(n_1, n_2) = \left\{ \frac{(Q \mp e)^2}{2C_\Sigma} - \left\{ n_1 e \left[\frac{C_G + C_2}{C_\Sigma} V - \frac{C_G}{C_\Sigma} V_G \right] + (n_2 \pm 1) e \left[\frac{C_1}{C_\Sigma} V + \frac{C_G}{C_\Sigma} V_G \right] \right\} \right\} - \left\{ \frac{Q^2}{2C_\Sigma} - \left\{ n_1 e \left[\frac{C_G + C_2}{C_\Sigma} V - \frac{C_G}{C_\Sigma} V_G \right] + n_2 e \left[\frac{C_1}{C_\Sigma} V + \frac{C_G}{C_\Sigma} V_G \right] \right\} \right\}$$

$$\Delta F_2^{\pm}(n_1, n_2) = \frac{e}{C_\Sigma} \left\{ \frac{e}{2} \mp Q \mp C_1 V \mp C_G V_G \right\} \tag{24}$$

By inserting $Q = Ne - Q_0$ into equation (24), the equation (2b) is obtained.

4. Master equation

Figure 4 shows the numerical simulation step to calculate IV curve based on Master equation method. First, the values of the physical constants (Boltzmann constant and elemental charge) and device parameters (C_1, C_2, C_G, R_1 and R_2) are defined. Then, the external parameters (V, V_G, Q_0 and T) are given. Next, the free energy change of the system ΔF when the electron tunnels across the tunnel capacitance, is calculated. The ΔF depends on the number of excess electrons N in the dot, as expressed in equations (23) and (24).

$$\Delta F_1^{\pm}(n_1, n_2) = \frac{e}{C_\Sigma}\left\{\frac{e}{2} \pm (Ne - Q_0) \mp (C_G + C_2)V \pm C_G V_G\right\} \tag{25a}$$

$$\Delta F_2^{\pm}(n_1, n_2) = \frac{e}{C_\Sigma}\left\{\frac{e}{2} \mp (Ne - Q_0) \mp C_1 V \mp C_G V_G\right\} \tag{25b}$$

Using the values of ΔF, single electron tunneling rates across each of two junctions is determined. Each rate depends on both the tunneling resistance of the junction and the total energy change of the system due to the tunneling event. On the other words, for single electron transistor circuit simulation, each electron tunneling has to be carefully monitored. The electron tunneling rate, which is represented by $\Gamma^{\pm}$, can be easily obtained from the basic golden-rule calculation (Averin & Lhikarev, 1991),

$$\Gamma_1^{\pm}(N) = \frac{1}{R_1 e^2}\left[\frac{-\Delta F_1^{\pm}}{1 - exp\left[\Delta F_1^{\pm}/k_B T\right]}\right] \tag{26a}$$

$$\Gamma_2^{\pm}(N) = \frac{1}{R_j e^2}\left[\frac{-\Delta F_2^{\pm}}{1 - exp\left[\Delta F_2^{\pm}/k_B T\right]}\right] \tag{26b}$$

Next, a stochastic process in SET circuit is considered. The island charge *e* will change by the tunneling of electrons from or to the island as described by the master equation.

$$\frac{\partial \rho(N,t)}{\partial t} = \rho(N+1)[\Gamma_2^{+}(N+1) + \Gamma_1^{-}(N+1)] - \rho(N)[\Gamma_2^{-}(N) + \Gamma_1^{+}(N)] \tag{27}$$

Here, the dc characteristics is investigated, therefore the steady state solution of equation (27) is desired. The steady state master equation is found by setting the time derivative of the probability distribution function equal to zero. Therefore, equation (27) becomes (Hanna et al., 1991)

$$\rho(N)[\Gamma_2^{-}(N) + \Gamma_1^{+}(N)] = \rho(N+1)[\Gamma_2^{+}(N+1) + \Gamma_1^{-}(N+1)]. \tag{28}$$

In this condition, it is necessary to calculate $\rho(N)$ for all of possible charge state *N*. By inserting *N* from $-\infty$ to ∞ into equation (28), the following equations are obtained.

$$\rho(-\infty)[\Gamma_2^{-}(-\infty) + \Gamma_1^{+}(-\infty)] = \rho(-\infty+1)[\Gamma_2^{+}(-\infty+1) + \Gamma_1^{-}(-\infty+1)]$$

$$\rho(-1)[\Gamma_2^{-}(-1) + \Gamma_1^{+}(-1)] = \rho(0)[\Gamma_2^{+}(0) + \Gamma_1^{-}(0)]$$

$$\rho(0)[\Gamma_2^{-}(0) + \Gamma_1^{+}(0)] = \rho(1)[\Gamma_2^{+}(1) + \Gamma_1^{-}(1)]$$

$$\rho(1)[\Gamma_2^-(1)+\Gamma_1^+(1)]=\rho(1)[\Gamma_2^+(2)+\Gamma_1^-(2)]$$

$$\rho(n)[\Gamma_2^-(n)+\Gamma_1^+(n)]=\rho(n+1)[\Gamma_2^+(n+1)+\Gamma_1^-(n+1)]$$

$$\rho(\infty-1)[\Gamma_2^-(\infty-1)+\Gamma_1^+(\infty-1)]=\rho(\infty)[\Gamma_2^+(\infty)+\Gamma_1^-(\infty)] \quad (29)$$

To solve equations above, the $\rho(n)$ must satisfy the standard boundary conditions, i.e.

$$\rho(N)\to 0, \text{ as } N\to\pm\infty. \quad (30)$$

Using this condition, all of the $\rho(N)$ can be found. However, the $\rho(N)$ here is not normalized, so that $\rho(N)$ requires the normalization as follows:

$$\sum_{N=-\infty}^{\infty}\rho(N)=1. \quad (31a)$$

For this, the following transformation is need.

$$\rho(N)\to\frac{\rho(N)}{\sum_{N=-\infty}^{\infty}\rho(N)} \quad (31b)$$

Finally, the current can be calculated by,

$$I(V)=e\sum_{N=-\infty}^{\infty}\rho(N)[\Gamma_1^+(N)-\Gamma_1^-(N)]. \quad (32a)$$

Here, the multiplication of the probability and the difference of rate $\Gamma_1^+(N)-\Gamma_1^-(N)$ describes the net current flowing through the first junction. In addition, the current may also expressed in the terms of the rates at second junction, as follows.

$$I(V)=e\sum_{N=-\infty}^{\infty}\rho(N)[\Gamma_2^+(N)-\Gamma_2^-(N)]. \quad (33b)$$

5. Matlab implementation

The above equations can be easily implemented in MATLAB. As explained in previous section, the flowchart of numerical simulation is as follows. In the first step, the following physical constant and device parameters are defined as follows.

```
% Matlab program source for numerical simulation of Master equation
% in single electron transistor
% This program code is made by Dr. Ratno Nuryadi, Jakarta, Indonesia
clear all;
% Definition of Physical constant
q=1.602e-19;            % electronic charge (C)
kb=1.381e-23;           % Boltzman constant (J/K)
% Definition of Device parameters
c1=1.0e-20;               % tunnel capacitor C1 (F)
c2=2.1e-19;               % tunnel capacitor C2 (F)
cg=1.0e-18;               % gate capacitor Cg (F)
ctotal=c1+c2+cg;          % total capacitance (F)
mega=1000000;             % definition of mega=10^6
r1=15*mega;               % tunnel resistance R1 (Ohm)
r2=250*mega;              % tunnel resistance R2 (Ohm)
```

Second, the values of external parameters (V, V_G, Q_0 and T) is given. Here, the V_G, Q_0 and T are kept a constant while the V is varied from V_{min} to V_{max}, as follows:

```
Vg=0;                    % gate voltage (V)
q0=0;                    % background charge q0 is assumed to be zero
temp=10;                 % temperature T (K)

vmin=-0.5;               % drain voltage minimum Vmin (V)
vmax=0.5;                % drain voltage maximum Vmax (V)
NV=1000;                 % number of grid from Vmin to Vmax
dV=(vmax-vmin)/NV;       % drain voltage increment of each grid point
for iv=1:NV              % loop start for drain voltage
V(iv)=vmin+iv*dV;        % drain voltage in each grid point
% Note that loop end for drain voltage is located in the end of this
program source
```

Third step is calculation of ΔF, as follows:

```
Nmin=-20;                % minimum number of N (charge number in dot)
Nmax=20;                 % maximum number of N (charge number in dot)
for ne=1:Nmax-Nmin       % loop start for N
    n=Nmin+ne;           % N charge number in dot
% Calculation of ΔF in equations (25a) and (25b)
    dF1p=q/ctotal*(0.5*q+(n*q-q0)-(c2+cg)*V(iv)+cg*Vg);
    dF1n=q/ctotal*(0.5*q-(n*q-q0)+(c2+cg)*V(iv)-cg*Vg);
    dF2p=q/ctotal*(0.5*q-(n*q-q0)-c1*V(iv)-cg*Vg);
    dF2n=q/ctotal*(0.5*q+(n*q-q0)+c1*V(iv)+cg*Vg);
% Noted that loop end for N is located after calculation of Γ
```

Forth, the values of ΔF are identified and then used for the calculation of Γ. If ΔF is negative, Γ will be calculated by equations (26a) and (26b(. However, if the ΔF is positive, Γ is set to be closed to the zero (very small). Note that the value of Γ is always positive. These identifications are done for four conditiond of ΔF.

```
    if dF1p<0
        T1p(ne)=1/(r1*q*q)*(-dF1p)/(1-exp(dF1p/(kb*temp)));
                          % Γ positive in equation (26a)
    else
        T1p(ne)=1e-1;     % Γ positive is assumed to be very small
    end
    if dF1n<0
        T1n(ne)=1/(r1*q*q)*(-dF1n)/(1-exp(dF1n/(kb*temp)));
                                    % Γ negative in equation (26a)
    else
        T1n(ne)=1e-1;       % Γ negative is assumed to be very small
    end
    if dF2p<0
        T2p(ne)=1/(r2*q*q)*(-dF2p)/(1-exp(dF2p/(kb*temp)));
                          % Γ positive in equation (26b)
    else
        T2p(ne)=1e-1;       % Γ positive is assumed to be very small
    end
```

```
    if dF2n<0
        T2n(ne)=1/(r2*q*q)*(-dF2n)/(1-exp(dF2n/(kb*temp)));
                                        % Γ negative in equation (26b)
    else
        T2n(ne)=1e-1;                   % Γ negative is assumed to
                                          be very small
    end
end                                     % loop end for N
```

Fiveth, the $\rho(N)$ of equation (28) is calculated. For this, normalization of equation (31a) must be satisfied. Here, the values of ρ(Nmin) and ρ(Nmax) is assumed to be 0.01.

```
p(1)=0.001;                         % ρ(N_min) is assumed to be 0.01
p(Nmax-Nmin)=0.001;                 % ρ(N_max) is assumed to be 0.01
```

Sixth, normalization of ρ is done. Here, $\sum_{N=-\infty}^{\infty}\rho(N)$ is calculated.

```
sum=0;                      % sum=0 is initial value to calculate ρ
for ne=2:Nmax-Nmin
    p(ne)=p(ne-1)*(T2n(ne-1)+T1p(ne-1))/(T2p(ne)+T1n(ne));
                            % calculation of ρ(N) in equation (28)
% The conditions below are used to avoid divergence of Matlab
calculation
    if p(ne)>1e250
        p(ne)=1e250;
    end
    if p(ne)<1e-250
        p(ne)=1e-250;
    end
% ----------------------
    sum=sum+p(ne);
end

for ne=2:Nmax-Nmin
    p(ne)=p(ne)/sum;        % Normalization in equation (31b)
end
```

Finally, the current is computed as follows:

```
sumI=0;                                 % sumI=0 is initial condition
                                          for current calculation
for ne=2:Nmax-Nmin
    sumI=sumI+p(ne)*(T2p(ne)-T2n(ne));
end
I(iv)=q*sumI;                           % I in equation (32b)
end                                     % end of drain voltage loop
plot(V,I);                              % plot of I vs V

for iv=1:NV-1
    dIdV(iv)=(I(iv+1)-I(iv))/dV;        % calculation of dIdV
end
figure;
plot(V(1,1:NV-1),dIdV);                 % plot of dIdV vs V
```

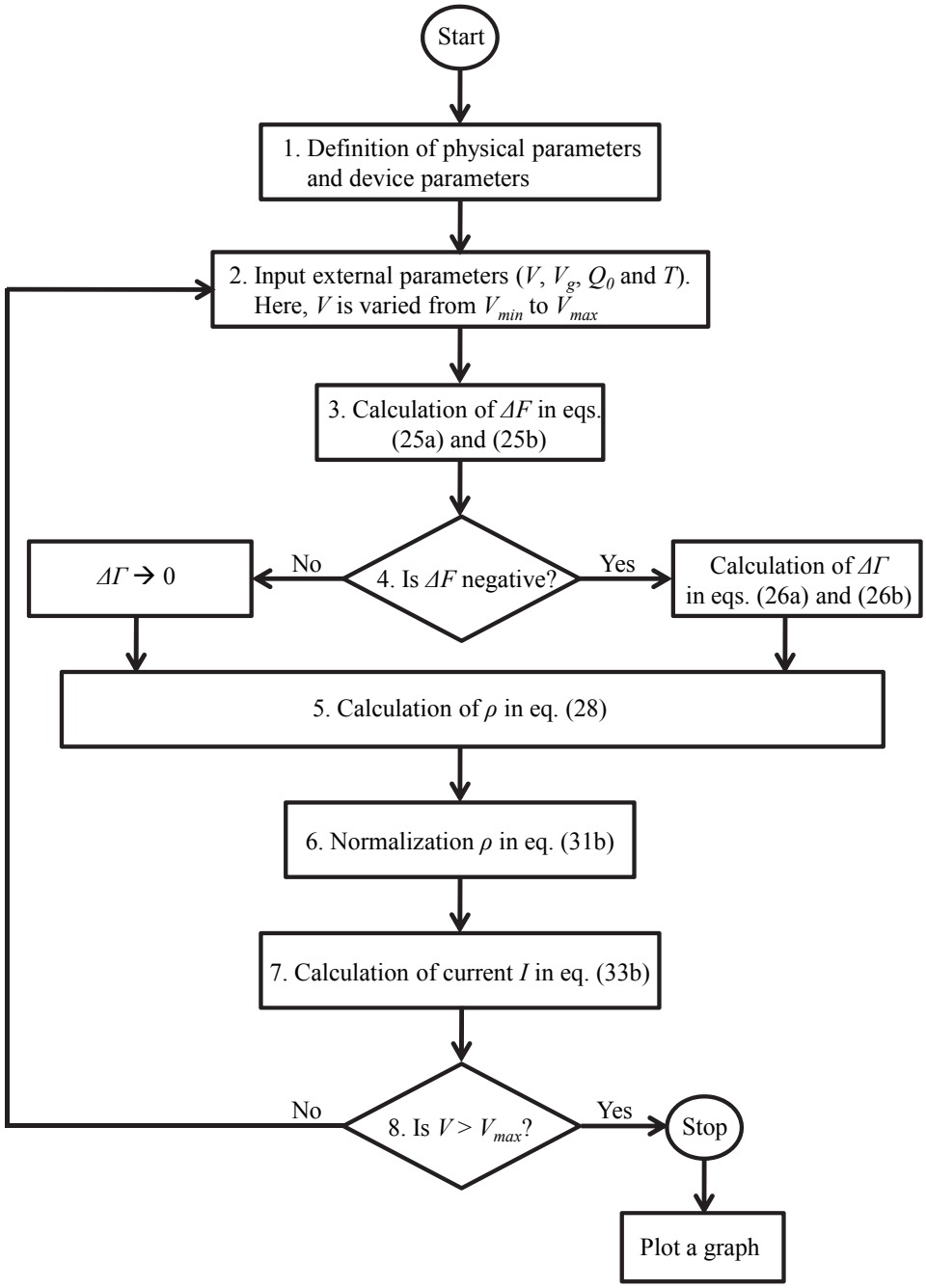


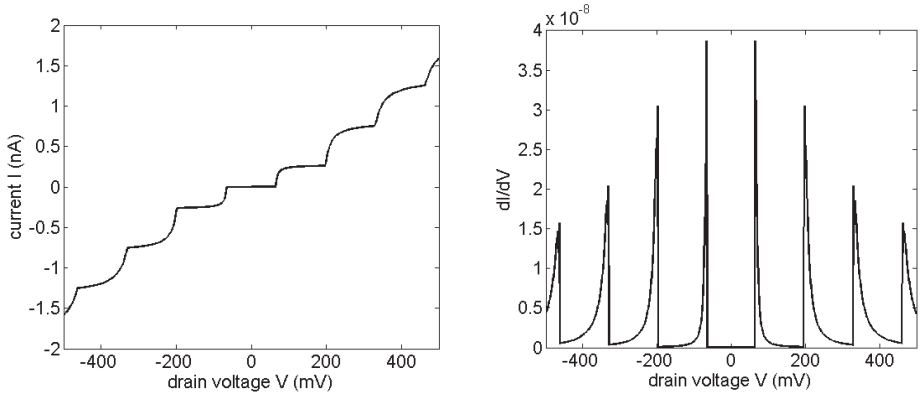
Fig. 4. Flow diagram of the Matlab program used to solve Master equation.

6. Examples of simulated results

Two examples will be used to demonstrate the numerical solution of Master equation in single electron transistor.

Example 1:

Figures 5(a) dan (b) shows current-drain voltage characteristic of the SET and its dI/dV curve. The parameter values are C_1= 1.0x10^{-20} F, C_2= 2.1x10^{-19} F, C_G= 1.0x10^{-18} F, R_1= 15 MΩ and R_2=250 MΩ. The calculation was carried out for an operating temperature of 10 K, V_G= 0 V and Q_0= 0. As shown in Fig. 5(a), at small source-drain voltage V there is no current, indicating the suppression of the current which is known as the Coulomb blockade. In this region, any tunneling event would lead to an increase of the total energy and also the tunneling rate is exponentially low. There is also evident that the I-V curve has staircase shape, which is called as Coulomb staircases.



(a) (b)

Fig. 5. (a) The current – drain voltage characteristics for SET and (b) dI/dV curve with the device parameters are C_1= 1.0x10^{-20} F, C_2= 2.1x10^{-19} F, C_G= 1.0x10^{-18} F, R_1= 15 MΩ, R_2=250 MΩ and the external parameters are V_G= 0 V and T=10 K.

The Coulomb staircase can be understood simply in terms of simulation model in equation (28). Initially at drain voltage V=0, we have ρ(N=0)=1, and $\Gamma_1^+(N=0)= \Gamma_2^+(N=0)=0$. When V=V$_t$ (V$_t$ is threshold voltage), the rates $\Gamma_1^+(N=0)$ and $\Gamma_2^+(N=0)$ jump sharply allowing charge to flow through the junction capacitances, so that ρ(n=1)>0. When V=V$_t$+e/2C$_\Sigma$ there is jump in $\Gamma_1^+(N=1)$ producing the next another step in I-V characteristics. Such steps happen due to each increase of V by e/2C$_\Sigma$. Simulation result in Fig. 5 has values of C_2>C_1 and R_2>R_1. According to Fig. 5(b), the width of the steps is ~131 mV, which is determined by e/2C$_\Sigma$.

Example 2:

The current-gate voltage characteristics of SET is plotted in Fig. 6. The parameter values are C_1= 4.2x10^{-19} F, C_2= 1.9x10^{-18} F, C_G= 1.3x10^{-18} F, R_1= 150 MΩ, R_2=150 MΩ, T=10 K and V= 10 mV. The program source for this I-V curve can be seen below, which is modified from the previous source.

```
V=0.01;                     % drain voltage (V)
q0=0;                       % background charge q0 is assumed to be
zero
temp=10;                    % temperature T (K)

vgmin=-0.4;                 % gate voltage minimum Vmin (V)
vgmax=0.4;                  % gate voltage maximum Vmax (V)
NVg=800;                    % number of grid from Vgmin to Vgmax
dVg=(vgmax-vgmin)/NVg;      % gate voltage increment of each grid point
for iv=1:NVg                % loop start for gate voltage
Vg(iv)=vgmin+iv*dVg;        % drain voltage in each grid point
% Note that loop end for drain voltage is located in the end of this
program source

Nmin=-20;                  % minimum number of N (charge number in dot)
Nmax=20;                   % maximum number of N (charge number in
dot)
for ne=1:Nmax-Nmin          % loop start for N
    n=Nmin+ne;              % N charge number in dot
% Calculation of ΔF in equations (25a) and (25b)
    dF1p=q/ctotal*(0.5*q+(n*q-q0)-(c2+cg)*V+cg*Vg(iv));
    dF1n=q/ctotal*(0.5*q-(n*q-q0)+(c2+cg)*V-cg*Vg(iv));
    dF2p=q/ctotal*(0.5*q-(n*q-q0)-c1*V-cg*Vg(iv));
    dF2n=q/ctotal*(0.5*q+(n*q-q0)+c1*V+cg*Vg(iv));
% Noted that loop end for N is located after calculation of Γ
```

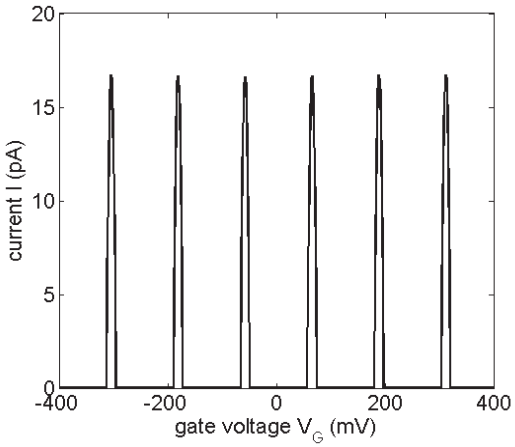


Fig. 6. The current – gate voltage characteristics for SET with the parameter values are C_1= 4.2x10^{-19} F, C_2= 1.9x10^{-18} F, C_G= 1.3x10^{-18} F, R_1= 150 MΩ, R_2=150 MΩ and T=10 K.The drain voltage is 10 mV.

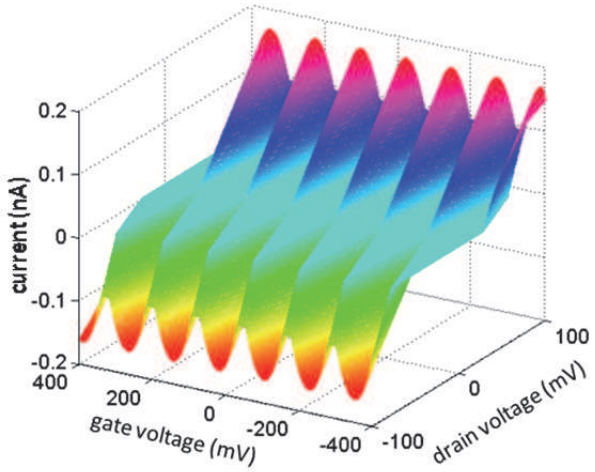


Fig. 7. 3D current – voltage characteristics for the SET. The range of source-drain voltage is from -100 mV to 100 mV and gate voltage is from -400 mV to 400 mV.

The current is a periodic function of the gate voltage V_G because the tunneling of one electron in or out of the dot is induced by the gate voltage. This periodic oscillations, which is also known as Coulomb oscillation, is the basis of the SET operation. In order to understand the overall of I-V characteristics, 3D plot is made as shown in Fig. 7. The Coulomb blockade region appears at very low source-drain voltage. The Coulomb blockade can be removed by the changing of gate voltage from inside Coulomb blockade to the outside. Outside the Coulomb blockade region, a current can flow the between the source and drain. At a given source-drain voltage V, the SET current can be modulated by gate voltage V_g. By sweeping the gate voltage, the currents oscillate between zero (Coulomb blockade) and non-zero (no Coulomb blockade), as shown in Fig. 6. The periodicity of the current is e/C_g along the gate voltage axis. Simulation results presented here reproduce the previous studies of the SET (Takahashi et al., 1995; Saitoh et al., 2001; Wolf et al., 2010; Sun et al., 2011; Lee et al., 2009), indicating that the simulation technique can be used to explain the basis of the SET.

7. Conclusion

This chapter has presented a numerical simulation of the single electron transistor using Matlab. This simulation is based on the Master equation method and is useful for both educational and research purposes, especially for beginners in the field of single electron devices. Simulated results produce the staircase behavior in the current-drain voltage characteristics and periodic oscillations in current-gate voltage characteristics. These results reproduce the previous studies of the SET, indicating that the simulation technique achieves good accuration. The resulting program can be also integrated into an engineering course on numerical analysis or solid-state physics.

8. References

Amman, M.; Wilkins, R.; Ben-Jacob, E.; Maker, P.D.; & Jaklevic, R.C. (1991). Analytic solution for the current-voltage characteristic of two mesoscopic tunnel junctions coupled in series, *Phys. Rev. B*, 43, pp. 1146-1149.

Averin, D.V. & Likharev, K.K. (1991). *Mesoscopic phenomena in Solids*, edited by B.L. Altshuler, P.A. Lee, and R.A. Webb (Elsevier, Amsterdam), pp. 173-271.

Fonseca, L.R.C.: Korotkov, A.N.: Likharev, K.K.; & Odintsov, A.A. (1997). A numerical study of the dynamics and statistics of single electron systems, *J. Appl. Phys.* 78 (5), pp. 3238-3251.

Hanna, A.E. & Tinkham, M. (1991). Variation of the Coulomb staircase in a two-junction system by fractional electron charge, *Phys. Rev. B*, 44, pp. 5919-5922.

Kirihara, M.; Kuwamura, N.; Taniguchi, K.; & Hamaguchi, C. (1994). Monte Carlo study of single-electronic devices, *Proceedings of the International Conference on Solid State Devices and Materials*, Yokohama, Japan, pp. 328-330.

Likharev, K.K. (1988). Correlated discrete transfer of single electrons in ultrasmall junctions, *IBM J. Res. Develop*. 32(1), pp. 144-157.

Likharev, K.K. (1999). Single-electron devices and their applications, *Proceedings of the IEEE*, 87, pp. 606-632.

Lee, D.S.; Yang, H.S.; Kang, K.C.; Lee, J.E.; Lee, J.H.; Park, S.H.; & Park, B.G. (2009). Silicon-Based Dual-Gate Single-Electron Transistors for Logic Applications", Jpn. J. Appl. Phys. 48, p. 071203.

Moraru, D.; Yokoi, K.; Nakamura, R.; Mizuno, T.; & Tabe, M. (2011). Tunable single-electron turnstile using discrete dopants in nanoscale SOI-FETs, *Key Engineering Materials*, 470, pp. 27-32.

Nuryadi, R.; Ikeda, H.; Ishikawa, Y.; & Tabe, M. (2003). Ambipolar coulomb blockade characteristics in a two-dimensional Si multidot device, *IEEE Trans. Nanotechnol.* 2, pp. 231-235.

Nuryadi, R.; Ikeda, H.; Ishikawa, Y.; & Tabe, M. (2005). Current fluctuation in single-hole transport through a two-dimensional Si multidot, *Appl. Phys. Lett*., 86, p. 133106.

Nuryadi, R.: & Haryono, A. (2010). Numerical simulation of single electron transistor using master equation, *Proc. SPIE (Southeast Asian International Advances in Micro/Nanotechnology)*, Vol. 7743, p. 77430L.

Ono, Y.; & Takahashi, Y. (2003). Electron pump by a combined single-electron/field-effect-transistor structure, *Appl. Phys. Lett.*, 82 (8), pp. 1221–1223.

Saitoh, M.; Saito, T.; Inukai, T.; & Hiramoto, T. (2001). Transport spectroscopy of the ultrasmall silicon quantum dot in a single-electron transistor, *Appl. Phys. Lett*., Vol. 79, No. 13, pp. 2025 - 2027.

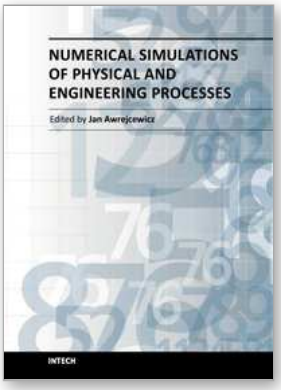
Sun, Y.; Rusli & Singh, N. (2011). Room-Temperature Operation of Silicon Single-Electron Transistor Fabricated Using Optical Lithography, *IEEE Trans. Nanotechnology*, 10(1), pp. 96-98.

Takahashi, Y.; Nagase, M.; Namatsu, H.; Kurihara, K.; Iwadate, K.; Nakajima, Y.; Horiguchi, S.; Murase, K. & Tabe, M. (1995). Fabrication technique Si single electron transistor operating at room temperature, *Electron. Lett.*, Vol. 31, No. 2, pp. 136–137.

Tucker, J.R. (1992). Complementary digital logic based on the "Coulomb blockade", *J. Appl. Phys.*, 72 (9), pp. 4399-4413.

Wasshuber, C.; Kosina, H.; & Selberherr, S. (1997). SIMON-A simulator for single-electron tunnel devices and circuits, *IEEE Transactions on Computer-Aided Design of Integrated Circuits and Systems*, 16 (9), pp. 937 – 944.

Wolf, C.R.; Thonke, K.; & Sauer, R. (2010). Single-electron transistors based on self-assembled silicon-on-insulator quantum dots, *Appl. Phys. Lett*. 96, p. 142108.



Numerical Simulations of Physical and Engineering Processes

Edited by Prof. Jan Awrejcewicz

ISBN 978-953-307-620-1
Hard cover, 594 pages
Publisher InTech
Published online 26, September, 2011
Published in print edition September, 2011

Numerical Simulations of Physical and Engineering Process is an edited book divided into two parts. Part I devoted to Physical Processes contains 14 chapters, whereas Part II titled Engineering Processes has 13 contributions. The book handles the recent research devoted to numerical simulations of physical and engineering systems. It can be treated as a bridge linking various numerical approaches of two closely inter-related branches of science, i.e. physics and engineering. Since the numerical simulations play a key role in both theoretical and application oriented research, professional reference books are highly needed by pure research scientists, applied mathematicians, engineers as well post-graduate students. In other words, it is expected that the book will serve as an effective tool in training the mentioned groups of researchers and beyond.

How to reference

In order to correctly reference this scholarly work, feel free to copy and paste the following:

Ratno Nuryadi (2011). Master Equation - Based Numerical Simulation in a Single Electron Transistor Using Matlab, Numerical Simulations of Physical and Engineering Processes, Prof. Jan Awrejcewicz (Ed.), ISBN: 978-953-307-620-1, InTech, Available from: http://www.intechopen.com/books/numerical-simulations-of-physical-and-engineering-processes/master-equation-based-numerical-simulation-in-a-single-electron-transistor-using-matlab

INTECH
open science | open minds

InTech Europe
University Campus STeP Ri
Slavka Krautzeka 83/A
51000 Rijeka, Croatia
Phone: +385 (51) 770 447
Fax: +385 (51) 686 166
www.intechopen.com

InTech China
Unit 405, Office Block, Hotel Equatorial Shanghai
No.65, Yan An Road (West), Shanghai, 200040, China
中国上海市延安西路65号上海国际贵都大饭店办公楼405单元
Phone: +86-21-62489820
Fax: +86-21-62489821