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

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## 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 & Likharev, 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 ( $h/4e^2 \approx 6.5 \text{ k}\Omega$ ). 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; Kirihaara 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 (Kirihaara 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 results 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 written as  $C_\Sigma$ , where

$$C_\Sigma = C_1 + C_2 + C_G. \quad (1)$$

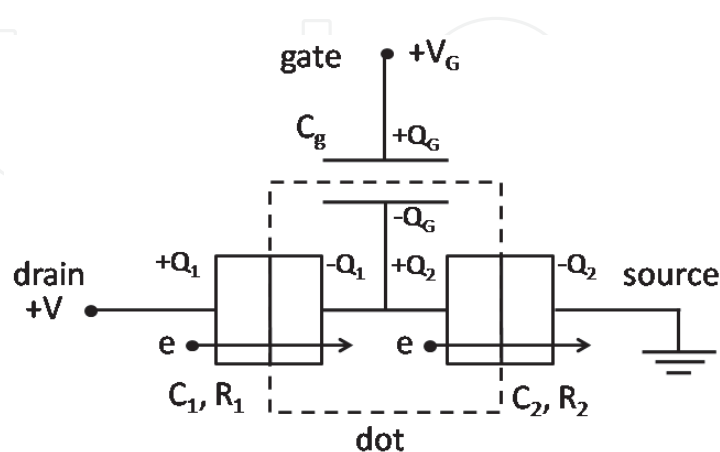


Fig. 1. Single electron transistor has a structure of the dot in the center coupled by two tunnel capacitors ( $C_1$  and  $C_2$ ) and a gate capacitor  $C_G$ . Source is connected to a ground, where drain and gate are applied by voltages  $V$  and  $V_G$  (Tucker, 1992).

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

*Free energy change:*

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

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

*Tunneling probability/rate:*

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

$$\Gamma_2^\pm(N) = \frac{1}{R_2 e^2} \left[ \frac{-\Delta F_2^\pm}{1 - \exp[\Delta F_2^\pm / k_B T]} \right] \quad (3b)$$

*Steady State Master equation:*

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

*Current equation:*

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

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  $n_2$  are a number of electrons flows through the capacitor  $C_1$  and capacitor  $C_2$ , respectively,  $Q_0$  is the background charge and  $\pm$  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  $\Delta F$  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  $\Delta F$  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  $\Gamma$  (i.e., probability per unit time) which depends solely on the  $\Delta F$ . 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 not. 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),

$$Q_1 = C_1 V_1 = C_1 (V - V_2), \quad (6a)$$

$$Q_2 = C_2 V_2, \quad (6b)$$

$$Q_G = C_G (V_G - V_2). \quad (6c)$$

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

$$Q = Q_2 - Q_1 - Q_G = Ne - Q_0. \quad (7)$$

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,

$$C_2 V_2 - C_1 (V - V_2) - C_G (V_G - V_2) = Q,$$

$$V_2 = \frac{1}{C_\Sigma} (C_1 V + C_G V_G + Q) \quad (8)$$

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,

$$V_1 = V - \frac{1}{C_\Sigma} (C_1 V + C_G V_G + Q)$$

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

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,

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

$$E_c = \frac{1}{2C_\Sigma} [C_G C_1 (V - V_G)^2 + C_1 C_2 V^2 + C_G C_2 V_G^2 + Q^2] \quad (10)$$

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).

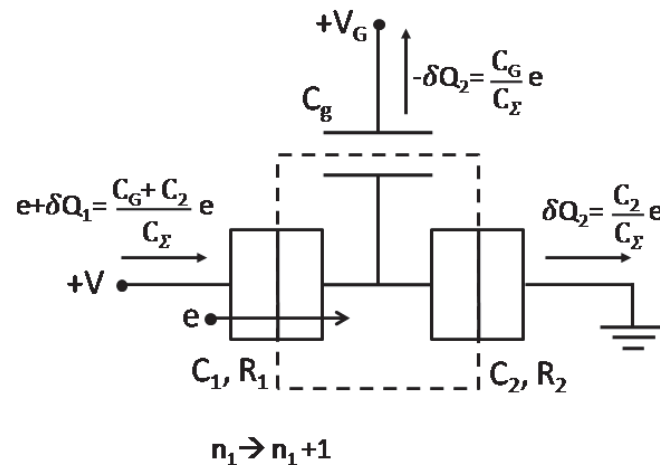


Fig. 3. The charge flow in the single electron transistor circuit when one electron through the capacitor  $C_1$  (Tucker, 1992).

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  $C_1$  ( $n_1 \rightarrow n_1 + 1$ )

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

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

$$\delta V_2 = \frac{e}{C_x} \quad (11)$$

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,

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

$$\delta Q_1 = -C_1 \delta V_2. \quad (12)$$

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

$$\delta Q_1 = -\frac{C_1}{C_x} e$$

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

$$\delta Q_1 + e = -\frac{C_1}{C_x} e + e$$

$$\delta Q_1 + e = \frac{C_2 + C_G}{C_x} e \quad (13)$$

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

$$\begin{aligned}\delta Q_2 &= C_2 V_2^{after} - C_2 V_2^{before}, \\ \delta Q_2 &= C_2 \delta V_2, \\ \delta Q_2 &= \frac{C_2}{C_x} e\end{aligned}\quad (14)$$

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

$$\begin{aligned}\delta Q_G &= C_G (V_G - V_2^{after}) - C_G (V_G - V_2^{before}), \\ \delta Q_G &= -C_G \delta V_2, \\ \delta Q_G &= -\frac{C_G}{C_x} e\end{aligned}\quad (15)$$

## 2. Work done when one electron tunnel through capacitor $C_1$ ( $n_1 \rightarrow n_1 + 1$ )

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,

$$\begin{aligned}W_S(n_1) &= n_1 [(e + \delta Q_1)V + (\delta Q_G)V_G + (\delta Q_2) \times 0], \\ W_S(n_1) &= n_1 \left[ \frac{C_G + C_2}{C_x} eV - \frac{C_G}{C_x} eV_G \right]\end{aligned}\quad (16)$$

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

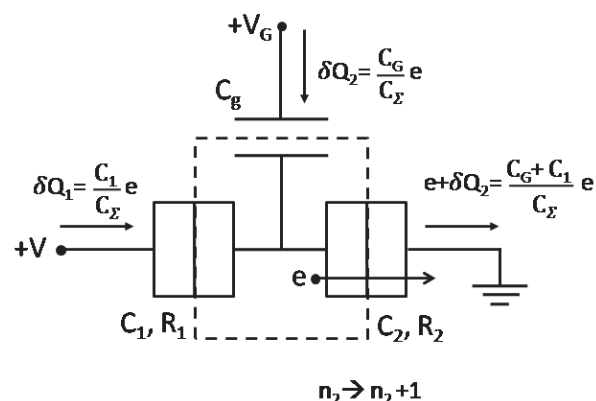


Fig. 3. The charge flow in the single electron transistor circuit when an electron tunnels through the capacitor  $C_2$ .

## 1. Change in charge when an electron through the capacitor $C_2$ ( $n_2 \rightarrow n_2 + 1$ )

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

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

$$\delta V_2 = -\frac{e}{C_S} \quad (17)$$

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

$$\begin{aligned} \delta Q_1 &= C_1(V - V_2^{after}) - C_1(V - V_2^{before}), \\ \delta Q_1 &= -C_1 \delta V_2, \\ \delta Q_1 &= \frac{C_1}{C_S} e \end{aligned} \quad (18)$$

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),  $\delta Q_2$  becomes,

$$\begin{aligned} \delta Q_2 &= C_2 V_2^{after} - C_2 V_2^{before}, \\ \delta Q_2 &= C_2 (\delta V_2), \\ \delta Q_2 &= -\frac{C_2}{C_S} e \end{aligned}$$

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

$$\begin{aligned} \delta Q_2 + e &= -\frac{C_2}{C_S} e + e, \\ \delta Q_2 + e &= \frac{C_1 + C_G}{C_S} e \end{aligned} \quad (19)$$

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

$$\begin{aligned} \delta Q_G &= C_G(V_G - V_2^{after}) - C_G(V_G - V_2^{before}), \\ \delta Q_G &= -C_G \delta V_2, \\ \delta Q_G &= \frac{C_G}{C_S} e \end{aligned} \quad (20)$$

## 2. Work done when one electron through the capacitor $C_2$ ( $n_2 \rightarrow n_2 + 1$ )

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

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

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



### 3.3 Free energy

The most important requirement for the occurrence of single electron tunneling is that the total energy of the transistor system must decrease due to one electron tunneling. In other words, 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:

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

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

### 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:

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

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

$$- \left\{ \frac{Q^2}{2C_\Sigma} - \left\{ n_1 e \left[ \frac{C_G + C_2}{C_\Sigma} V - \frac{C_G}{C_\Sigma} V_G \right] + n_2 e \left[ \frac{C_1}{C_\Sigma} V + \frac{C_G}{C_\Sigma} V_G \right] \right\} \right\}$$

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

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:

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

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

$$- \left\{ \frac{Q^2}{2C_\Sigma} - \left\{ n_1 e \left[ \frac{C_G + C_2}{C_\Sigma} V - \frac{C_G}{C_\Sigma} V_G \right] + n_2 e \left[ \frac{C_1}{C_\Sigma} V + \frac{C_G}{C_\Sigma} V_G \right] \right\} \right\}$$

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

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  $\Delta F$  when the electron tunnels across the tunnel capacitance, is calculated. The  $\Delta F$  depends on the number of excess electrons  $N$  in the dot, as expressed in equations (23) and (24).

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

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

Using the values of  $\Delta F$ , 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 & Likharev, 1991),

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

$$\Gamma_2^\pm(N) = \frac{1}{R_2 e^2} \left[ \frac{-\Delta F_2^\pm}{1 - \exp[\Delta F_2^\pm / k_B T]} \right] \quad (26b)$$

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.

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

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)

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

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

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

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

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

$$\begin{aligned}
\rho(1)[\Gamma_2^-(1) + \Gamma_1^+(1)] &= \rho(1)[\Gamma_2^+(2) + \Gamma_1^-(2)] \\
\rho(n)[\Gamma_2^-(n) + \Gamma_1^+(n)] &= \rho(n+1)[\Gamma_2^+(n+1) + \Gamma_1^-(n+1)] \\
\rho(\infty-1)[\Gamma_2^-(\infty-1) + \Gamma_1^+(\infty-1)] &= \rho(\infty)[\Gamma_2^+(\infty) + \Gamma_1^-(\infty)]
\end{aligned} \tag{29}$$

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

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

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:

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

For this, the following transformation is need.

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

Finally, the current can be calculated by,

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

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.

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

## 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=106
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  $\Delta F$ , 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  $\Delta F$  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  $\Gamma$ 
```

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

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

```

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

```

Fifth, the  $\rho(N)$  of equation (28) is calculated. For this, normalization of equation (31a) must be satisfied. Here, the values of  $\rho(N_{\min})$  and  $\rho(N_{\max})$  is assumed to be 0.01.

```

p(1)=0.001;
p(Nmax-Nmin)=0.001;
                                %  $\rho(N_{\min})$  is assumed to be 0.01
                                %  $\rho(N_{\max})$  is assumed to be 0.01

```

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

```

sum=0;
                                % sum=0 is initial value to calculate  $\rho$ 
for ne=2:Nmax-Nmin
    p(ne)=p(ne-1)*(T2n(ne-1)+T1p(ne-1))/(T2p(ne)+T1n(ne));
                                % calculation of  $\rho(N)$  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 of drain voltage loop
                                % plot of I vs V
plot(V,I);

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

```

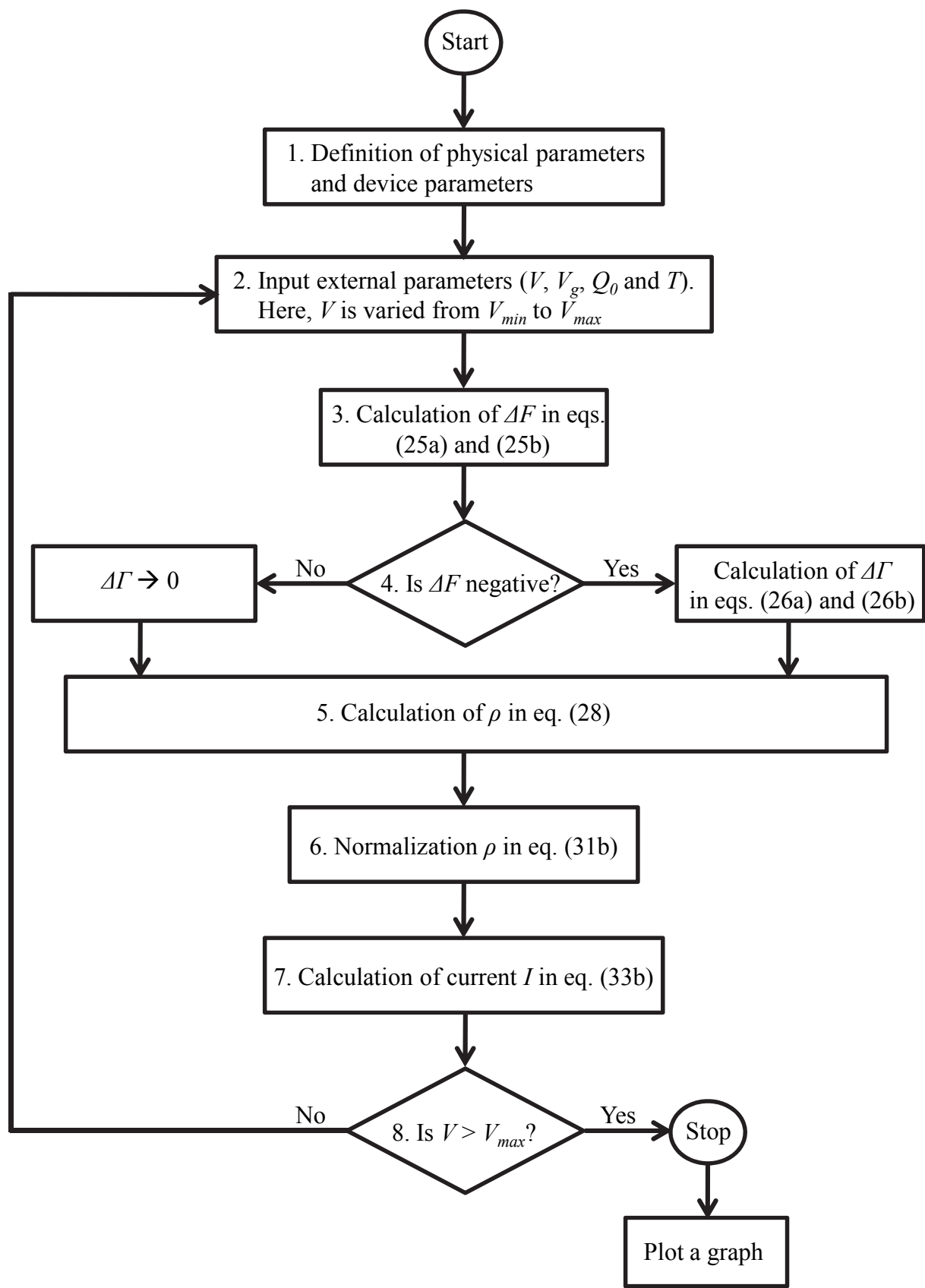


Fig. 4. Flow diagram of the Matlab program used to solve Master equation.

## 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) and (b) show current-drain voltage characteristic of the SET and its  $dI/dV$  curve. The parameter values are  $C_1 = 1.0 \times 10^{-20}$  F,  $C_2 = 2.1 \times 10^{-19}$  F,  $C_G = 1.0 \times 10^{-18}$  F,  $R_1 = 15$  M $\Omega$  and  $R_2 = 250$  M $\Omega$ . 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.

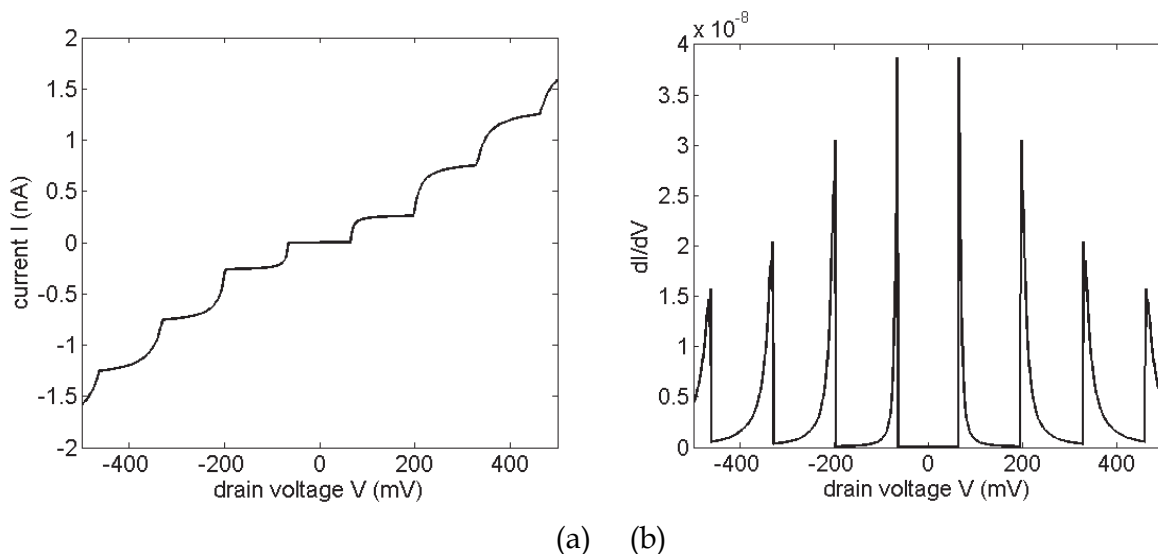


Fig. 5. (a) The current - drain voltage characteristics for SET and (b)  $dI/dV$  curve with the device parameters are  $C_1 = 1.0 \times 10^{-20}$  F,  $C_2 = 2.1 \times 10^{-19}$  F,  $C_G = 1.0 \times 10^{-18}$  F,  $R_1 = 15$  M $\Omega$ ,  $R_2 = 250$  M $\Omega$  and the external parameters are  $V_G = 0$  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  $\rho(N=0)=1$ , 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  $\rho(n=1)>0$ . 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  $\sim 131$  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  $C_1 = 4.2 \times 10^{-19}$  F,  $C_2 = 1.9 \times 10^{-18}$  F,  $C_G = 1.3 \times 10^{-18}$  F,  $R_1 = 150$  M $\Omega$ ,  $R_2 = 150$  M $\Omega$ ,  $T = 10$  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  $\Delta F$  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  $I$ 

```

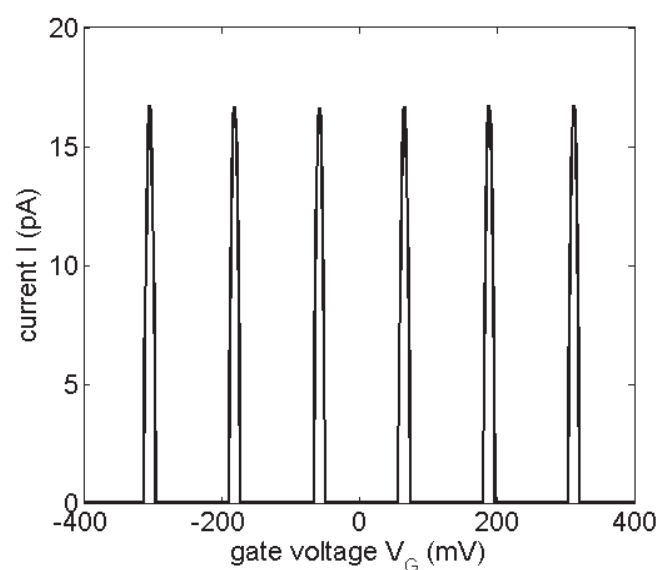


Fig. 6. The current - gate voltage characteristics for SET with the parameter values are  $C_1=4.2 \times 10^{-19}$  F,  $C_2=1.9 \times 10^{-18}$  F,  $C_G=1.3 \times 10^{-18}$  F,  $R_1=150$  M $\Omega$ ,  $R_2=150$  M $\Omega$  and  $T=10$  K. The drain voltage is 10 mV.



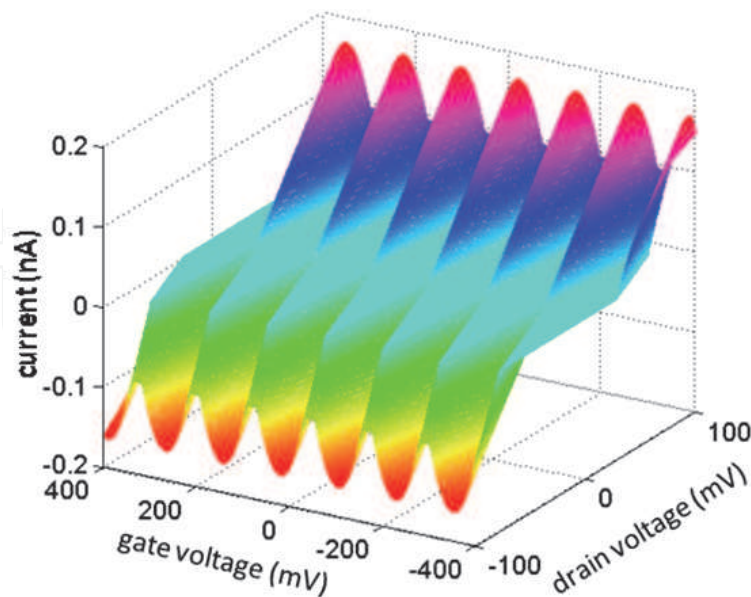


Fig. 7. 3D current – voltage characteristics for the SET. The range of source-drain voltage is from -100 mV to 100 mV and gate voltage is from -400 mV to 400 mV.

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 accuracy. The resulting program can be also integrated into an engineering course on numerical analysis or solid-state physics.

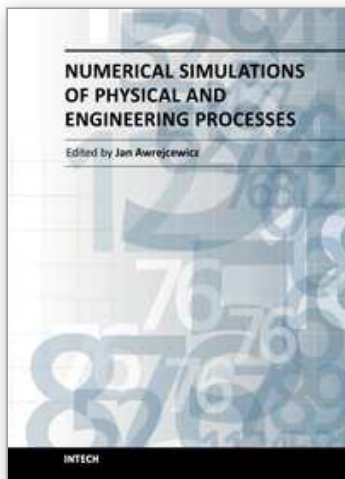
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## **Numerical Simulations of Physical and Engineering Processes**

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