

Simulation and Modeling of Silicon Based Single Electron Transistor

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ABSTRACT

In this work, we simulated and modeled silicon quantum dot based single electron transistor (SET). We simulated the device using non-equilibrium Green's function (NEGF) formalism in transport direction coupled with Schrodinger equation in transverse directions. The characteristics of SET such as Coulomb blockade and Coulomb diamonds were observed. We also present a new efficient model to calculate the current voltage (IV) characteristics of the SET. The IV characteristic achieved from the model are very similar to those from simulations both in shape and magnitude. The proposed model is capable of reproducing the Coulomb diamond diagram in good agreement with the simulations. The model, which is based on transmission spectrum, is simple, efficient and provides insights on the physics of the device. The transmission spectrum at equilibrium is achieved from simulations and given as input to the model. The model then calculates the evolved transmission spectra at non-equilibrium conditions and evaluates the current using Landauers formula.

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1. INTRODUCTION

The CMOS technology is at the verge of the miniaturization and it needs to be replaced by the new technologies which should overcome its limitations. One of the most promising technologies is the one based on single electron tunneling phenomenon. If a metallic or semiconducting island is placed between the electrodes separated by the tunnel junctions with very small capacitance, the single electron phenomenon can be observed. When an electron tunnels into the island it raises the electrostatic potential of island stopping the tunneling of the following electrons until external potential is applied. This phenomenon is also known as Coulomb blockade. If the island size is very small (so that the capacitance is very small), tunneling of single electrons can be controlled by the external electrode potentials. Hence the devices based on single electron phenomenon have the attributes of small size and low power consumption.

Over the years, many different schemes for digital logic using single electron transistor have been presented [1–5]. In one scheme, the logic states are represented by the single electrons located at tiny metallic electrodes [1]. While such a scheme can provide the huge benefits in terms of high speed and very low power consumption, its practical implementation faces serious challenges. Firstly, they should be operated at temperature much less than the critical temperature, otherwise a thermally induced tunneling event can change the entire calculation. Secondly, the output of one logic gate (single electron) should be capable of charging the input of following gates. This requires the stray capacitance of interconnections to be kept negligible and complicated design rules for different number of subsequent gates [2].

Single electron transistors (SET) based on silicon have been previously studied in [6–8]. In order to operate the transistor at room temperature, the size of the island should be less than 5nm [9]. The nano-lithography techniques now a days allow to define such small structures with only a few variations. In this work, we simulate and model the SET based on silicon quantum dot with a size of 1nm. We present two novel contributions in this work. i) We

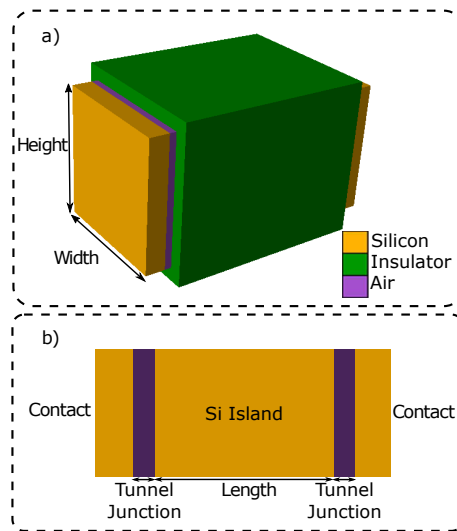


Figure 1. a) The three-dimensional structure of the device which is simulated in Atlas TCAD b) Cross section of the same device as seen from the sides. Different materials and the dimensional parameters are highlighted and drain and source contacts are mentioned. The gate contact is all around the device.

simulate Si based SET, for the first time, using Atlas TCAD [10] with non-equilibrium Green's function (NEGF) technique. The results are comparable to the experimental results with similar devices. NEGF formalism is a robust technique for the quantum level simulations. Anantram et. al used NEGF technique to model nanodevices [11]. The transport through quantum dot weakly coupled with the contacts is studied using NEGF technique in [12]. ii) We propose transmission spectrum based model for the evaluation of SET characteristics. The proposed model, which is the extended version of [13], uses transmission spectrum to calculate the current. It does not need any complex initial set up and is very efficient, simple, sufficiently accurate and flexible to implement in different conditions. In comparison, Monte Carlo based models [14] are accurate but very time consuming. Macromodeling based models [15] [16] are efficient but provide a little physical insights on the device behavior. Analytical models based on physics [17] and master equation [18] solve this problem but they still require a complex procedure to calculate tunnel junction resistances and capacitances [19]. These models require the tunnel junction resistances and capacitances as input while the proposed model requires transmission spectrum as input. The transmission spectrum provides insights on the physics of device especially about the density of states of island which lacks in case of other models. We can easily change the model for the variations in contact coupling, gate coupling and density of state variations due to different fabricated size of island. From the transmission spectrum current is calculated using Landauers formula. The rest of the paper is organized as follows. In section II the explanation of the device and simulations are described. In section III the details of proposed model are given. In section IV the results are discussed and the section V concludes the paper.

2. SIMULATIONS OF THE DEVICE

We simulated the single electron transistor (SET) based on silicon island and the drain and source contacts made of highly doped silicon (Fig. 1). The cross section of the island (height into width) is $1 \times 1 \text{ nm}$ and the length is 2 nm . The tunnel junctions are created by the gap between the island and contacts. These gaps provide the confinement in the transport direction and decouple the island from electrodes. The silicon island is warped by the oxide through which gate contact controls the conduction in the island. The device works as the single electron transistor and shows the characteristics of SET such as Coulomb diamonds as shown in results section. We simulated the device in Atlas TCAD using non-equilibrium Green's function (NEGF) formalism in transport direction coupled with Schrodinger equation in transverse direction. The simulator uses mode space technique instead of solving 2d or 3d problem. First solving the Schrodinger equation eigenvalues and eigen vectors are calculated in each slice of device. Then a transport equation is solved for electrons moving in lowest sub-bands which are occupied. This reduces the size of the problem [10]. But still the simulations are very time consuming and there is a need for an efficient model. From the simulations, we can achieve the transmission spectrum (TS) at equilibrium which is fed to the model to compute the IV characteristics. The IV characteristics are also calculated from the simulations to compare with those from the model.

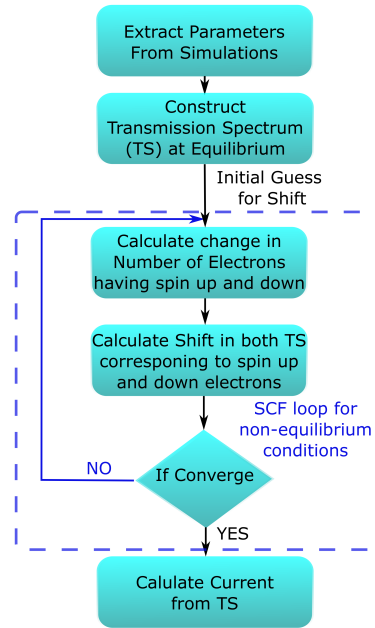


Figure 2. The flow chart of the model: at equilibrium, the transmission spectrum is constructed using parameters from simulations, while at non-equilibrium conditions, shift is calculated by the self-consistent loop.

3. THE MODEL

The proposed model uses transmission spectrum (TS) to calculate the characteristics of single electron transistors. In our previous works, we have implemented earlier versions of the model to molecular devices [20] and silicon nanocrystals [13]. The current model is implemented on SET and the difference from [20] is the implementation of two spectra for different spin as explained in [13]. In this work, we extend the model presented in [13] to implement the gate voltage in order to use the silicon nanocrystal as SET. Further explanation on the modeling of gate voltage can be found in the following description and in the results section. The model takes as input the transmission spectrum at equilibrium from the simulations. From the transmission spectrum, current is calculated using Landauers formula. The evolution in transmission spectrum with applied voltage is calculated by the model using self-consistent field technique. By evaluating the TS at all voltages (V_{ds} , V_g) and using the Landauers formula, IV characteristics of the device can be calculated [21].

We calculate the TS at equilibrium using Atlas TCAD. The TS parameters i.e. position, amplitude and width of peaks are given as input to the model. The model uses these parameters to construct the TS at equilibrium. The shape of the peaks is defined by the Lorentzian function.

$$D_0 = k_0 \times Norm\left(\frac{\gamma_1 \gamma_2}{(E - \epsilon)^2 + \gamma^2}\right) \quad (1)$$

Here D_0 is the transmission peak defined over the range of energies E , ϵ is the position of the corresponding peak and γ is the sum of drain and source rate constants γ_1, γ_2 . The width (or broadening) of the transmission peaks is defined by γ . After normalizing the Lorentzian function, it is multiplied by the amplitude of the corresponding peak k_0 . Other peaks are calculated similarly and then TS is constructed by adding all the transmission peaks. The same procedure is repeated for both spins and two spectra are achieved. Although at this point both the spectra are similar, the difference arises when the shift in spectra is calculated as explained below.

When the voltage is applied, transmission spectrum shifts on the energy axis. The shift is caused by the external potential and because of the change in number of electrons. At equilibrium, the Fermi level of island is aligned with the drain and source chemical potential. When the drain to source voltage (V_{ds}) is applied the drain and source chemical potential split and the separation is so called bias window. If there is a transmission peak inside or at the edge of the bias window then the number of electrons (N) at the island change. If the transmission peak corresponds to the spin up electrons the change in number of electrons are calculated using following formula.

$$N_{UP/DN} = \frac{\gamma_1 f_{1UP/DN}(\epsilon) + \gamma_2 f_{2UP/DN}(\epsilon)}{\gamma_1 + \gamma_2} \quad (2)$$

Here $f_{1UP/DN}(\epsilon)$ and $f_{2UP/DN}(\epsilon)$ are the drain and source Fermi functions with respect to the corresponding spin up/down transmission peaks (ϵ). If the number of electrons increase in the island the energy of the system increases so the transmission spectrum shifts towards higher energies and vice versa. The overall shift is the result of both i.e. change in number of electrons and the applied drain to source bias. The positive gate voltage lowers the energy of the island so it shifts the transmission spectrum towards low energies. The overall shift (U) can be calculated using:

$$U_{UP/DN} = U_L + U_0 \Delta N_{DN/UP} \quad (3)$$

where U_0 is the single electron charging energy, $\Delta N_{DN/UP}$ is the change in number of spin down/up electrons and $U_L = \alpha_d V_{ds} + \alpha_g V_g$ is Laplace potential. The effect of the external voltages is modeled by the coupling coefficients α_d, α_g . Equation 2 and 3 are solved self-consistently to calculate the shift in transmission spectrum with respect to the applied voltage. The shift in both the spectra for spin up and spin down is calculated. The shift in the spin up transmission spectrum is calculated from the change in number of spin down electrons as spin up electron feels the potential due to spin down electron and vice versa [21].

When a positive gate voltage is applied and a lowest unoccupied molecular level (LUMO) goes below the drain and source chemical potentials, the number of electrons increase on the island. This increase in number of electrons causes the rate constant (γ) to decrease so the width of the transmission peaks also reduces. In the current version of the model, the change in width is calculated using fitting parameters. Another effect of the increase in number of electrons on the island is to reduce the gate coupling (α_g). With the increase in number of electrons on the island the amount of shift in transmission spectra due to increase in gate voltage reduces. We implement this effect in the model by linear fitting of α_g with respect to the change in number of electrons (N). After evaluating the transmission spectra evolved with the applied voltage we can find the current using Landauers formula.

$$I_{UP/DN} = \frac{q^2}{h} \int_{-\infty}^{+\infty} T_{UP/DN}(E) [f_1(E) - f_2(E)] dE \quad (4)$$

Here q is the electron charge, h is plank's constant and $T(E)$ is the transmission spectrum. The difference between the source and drain Fermi functions models the effect of bias window so that only the part of transmission spectrum

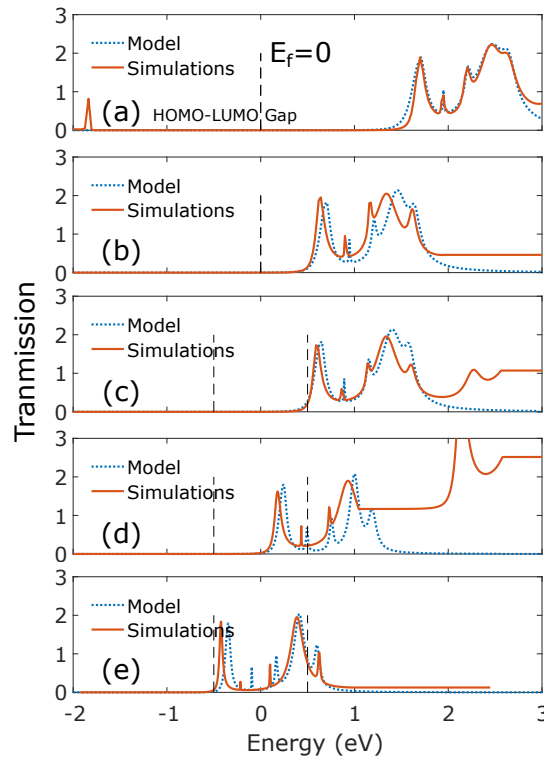


Figure 3. Transmission spectra at different V_g and V_{ds} achieved from simulations and model. The bias window is shown as the dashed lines. a) $V_g = 0.0V$, $V_{ds} = 0.0V$ b) $V_g = 1.0V$, $V_{ds} = 0.0V$ c) $V_g = 1.0V$, $V_{ds} = 1.0V$ d) $V_g = 1.5V$, $V_{ds} = 1.0V$ e) $V_g = 2.5V$, $V_{ds} = 1.0V$.

which is inside the bias window is integrated. The total current is calculated by the sum of spin up and spin down currents.

4. RESULTS AND DISCUSSION

Single electron transistor based on silicon quantum dot of 1nm cross section was simulated in Atlas TCAD using NEGF formalism coupled with Schrodinger equation. The IV characteristics of the device were calculated from simulations as well as from the model. In Fig. 3 the transmission spectra (TS) from simulations and model are shown for different values of V_g and V_{ds} . The lowest unoccupied molecular levels (LUMO) are shown while the highest occupied molecular levels (HOMO) are not shown because they do not contribute to the conduction in this case as they are far below the Fermi energy level ($E_f = 0$). The HOMO-LUMO gap and the Fermi energy level are also mentioned in the Fig. 3 (a). The LUMO levels are relatively closer to Fermi level and by applying a positive gate voltage we can shift them near Fermi level (Fig. 3 (b)). Then at a small value of V_{ds} LUMO1 enters inside the bias window and contributes to current (Fig. 3 (c,d,e)).

The comparison between the IV characteristics is shown in the Fig. 4. Drain current is plotted as a function of drain to source bias for different values of gate voltage. At low gate voltages (i.e. less than 1 V) there are no transmission peaks inside the bias window so a very small current flows through device because of tunneling of electrons with very low probability. The model provides acceptable estimation of the current as shown in the figure in case of $V_g = 0.7, 0.8, 0.9, 1.0V$. The first peak starts to enter in the bias window at $V_g = 1V$ as shown in the Fig. 3 (c).

The current is modeled very effectively at the gate voltages higher than 1V (Fig. 4) because the bias window, for the selected range of V_{ds} , includes the transmission peaks. As the model is transmission spectrum based so the results are better when there is a transmission peak inside the bias window. For the sake of clarity, the different curves shown here are selected in such a way that they do not overlap each other. In Fig. 5 (a) the IV characteristics for both positive and negative drain to source bias are shown for $V_g = 2.0V$. This shows that our model is valid for bidirectional electron flow. And in the Fig. 5 (b) the results from the previous model without considering the spin of electron (Model w/o Spin) is compared with the proposed model (Model w Spin) under the same conditions and parameters. We can see that the proposed model provides very accurate results compared to the previous version of the model in [20].

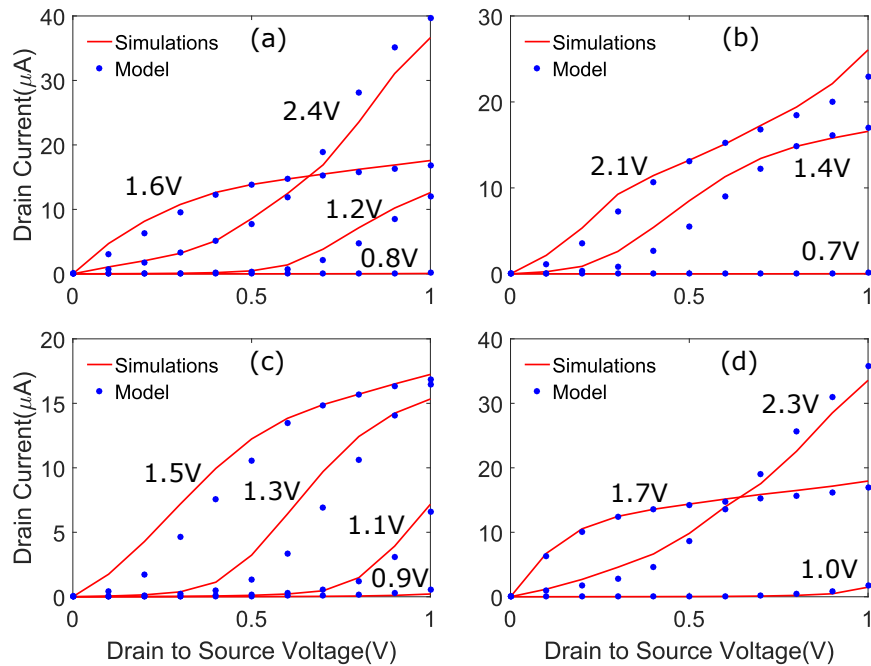


Figure 4. Comparison of IV characteristics of the device at various gate voltages between the model and simulations. Different curves are for different gate voltages mentioned by the curves. At lower gate voltages, less than 1.0V, there are no peaks inside the bias window. First peak enters in the bias window at $V_g = 1.1V$ so a high current flows. As the gate voltage increases other peaks also contribute to the current.

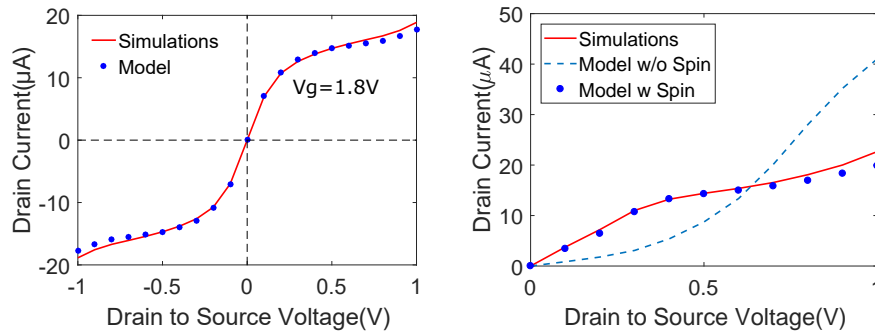


Figure 5. a) IV characteristics of the simulated device at gate voltage equal to 1.8V and for both positive and negative drain to source bias. b) IV characteristics obtained from the previous model without considering the spin and from the current model with the different spectra for spin at $V_g = 2.0V$.

The current as a function of V_{ds} and V_g is plotted on grayscale in Fig. 6. The magnitude of the current is represented by the shade of the gray according to the scale shown in the figure. The dark regions represent the zero or very small current while the current of higher magnitudes is represented by the light regions. The coulomb blockade diamonds which are unique characteristics of SET can be seen in the form of dark regions. One large blockade diamond and one small one can be observed in the figure. The model successfully predicts the same behavior as obtained from simulations. The resolution of the plots in Fig. 6 (a,b) is not good and it would take high computational effort to increase it in case of simulations. We have shown the high resolution achieved from the model in Fig. 6 (c). The time required for the calculations in Fig. 6 (a,b) is 6346s by the TCAD simulations and 1.57s by the model. The model takes 128s for the calculation with high resolution plot (210 V_{ds} points and 260 V_g points) Fig. 6 (c). All the

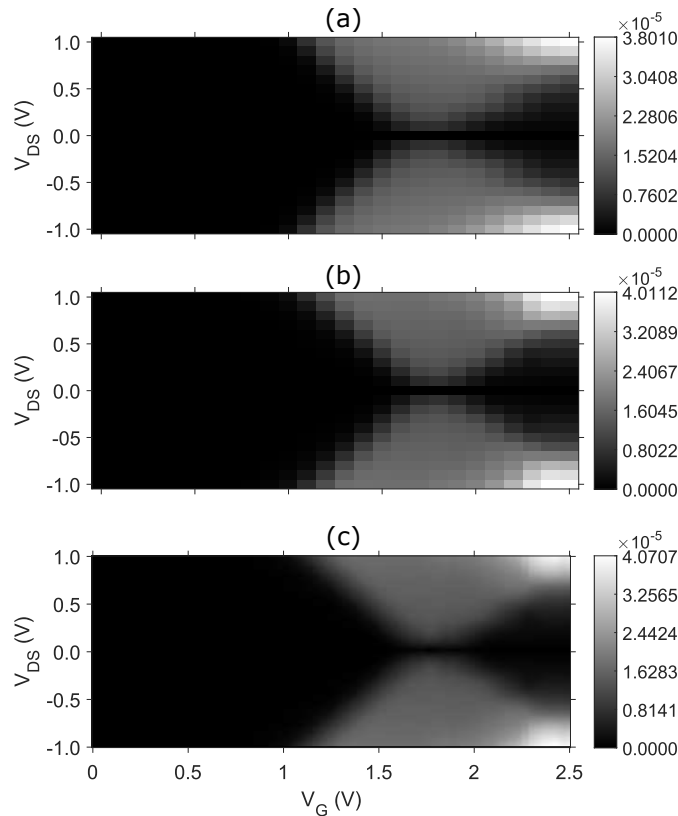


Figure 6. The current plotted as a function of V_{ds} and V_g . The shade of greyscale represents the drain current value based on the scale shown in the figure. The three figures are obtained from a) simulations b) model c) model using refined set of applied voltages.

simulations were performed on the same system with the Intel core i5 1.8 GHz processor and 6 GB of RAM. The proposed model provides sufficiently accurate results while maintaining the efficiency. While other compact models based on macromodeling are also efficient, the proposed model captures the physical information of device with more details.

5. CONCLUSIONS

In this work, we simulated and modeled the single electron transistor based on silicon quantum dot. We simulated the device in Atlas TCAD using NEGF formalism in transport direction coupled with Schrodinger equation in transverse direction. The SET characteristics such as Coulomb blockade and Coulomb diamonds were observed in the results obtained from the simulations and the model. The IV characteristics of the SET were obtained from the model having a good agreement with the simulations. The proposed model is simple, efficient, flexible and provides insights on the physics of the device. In the future, we will include in the model the effect of the change in number of electrons on the width of the transmission peaks. We will also use the device for circuit level implementation.

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