

A Model of a Single Electron Transistor of Metallic Tunneling Junctions and Its Validation *

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Abstract : Based on the orthodox theory ,a model of a single electron transistor (SET) of metallic tunneling junctions is built using the master equation method. Several parameters of the device ,such as capacitance ,resistance and temperature ,are input into the model and thus the I - V curves are attained. These curves are consistent with those from other experiments ;therefore ,the model is verified. However ,there still exists a difference between simulated results and experimental results ,mainly comes from the stationary case of the master equation. In other words ,precision of simulated results would be increased if the transient case of the master equation is considered. Moreover ,the current increases exponentially at higher drain voltages ,which is due to the fact that the barrier suppression is caused by the image charge potential.

Key words : single electron transistor ; orthodox theory ; coulomb blockade ; quantum tunnelling

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1 Introduction

For its low-power ,high-speed ,high-sensitivity propriety ,single electron transistors (SET) have received a lot of attention from specialists and scholars. In the 1980s ,Averin and Likharev found the orthodox theory of a single electron system which can quantificational by describing the phenomenon of single electron tunneling^[1,2]. Recently ,with the rapid development of micro-fabrication technology ,islands in nanometer scale have been successfully manufactured using different methods^[3~5]. On the basis of these small islands ,SET can be manufactured. Characteristic curves of SET can be measured in very low temperatures ,usually several K or hundreds of mK. At a given temperature ,whether the Coulomb phenomenon can be observed is determined by the size of the island.

The purpose of this paper is to build a mathematic model of SET and to test its veracity by comparing the curves from simulations with those from other experiments.

2 Model

2.1 Orthodox theory

The model in this paper is based on the orthodox theory which describes the charge transmission in the Coulomb blockade situation. In this theory , tunneling Hamiltonian H_T is treated as a weak perturbation to the system H_0 and is calculated using the perturbation approximation method. Considering the change in free energy ,as well as according to Fermi 's golden rule ,the tunneling rate from the initial state i to the final state f is given by^[6,7]

$$\Gamma_{if}(F) = \frac{2}{\hbar} |T_{if}|^2 (E_i - E_f - F) \quad (1)$$

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where $|T_{if}|$ is the tunnel transmission coefficient, and F is the increase of system free energy. It is reasonable to make approximations by neglecting the variation of the tunnel transmission coefficient with energy and momentum. Using the density of states $D(E)$, the number of electron states in a small energy interval dE is given by $D(E)dE$ and the density of states can be treated as a constant. For a metallic tunnel junction, the Fermi level lies well on the conduction band and the tunnel rate of the electron which can be described as

$$\Gamma(F) = \frac{e^2 R_T}{2} \frac{F}{k_B T} \exp\left(-\frac{F}{k_B T}\right) \quad (2)$$

where R_T is the tunneling resistance given by

$$R_T = \frac{\hbar}{2 e^2 |T|^2 D_i D_f} \quad (3)$$

2.2 Calculation of free energy

Free energy is an important parameter in a single electron system. Only the tunneling that causes free energy to decrease can occur, otherwise there will be no electron tunneling. Figure 1 shows the circuit diagram of the metallic tunnel junction SET with gate voltage V_g ^[8].

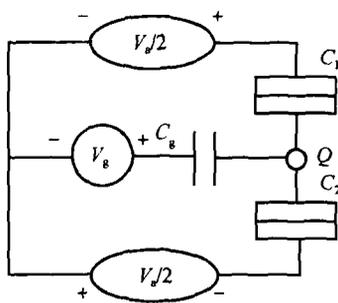


Fig. 1 Equivalent circuit diagram of the SET with gate voltage V_g

The island Q is located between two tunnel junctions whose capacity and resistance are C_1 and R_1 , C_2 and R_2 , respectively. C_g is the gate capacitance. When the island possesses N electrons, the change of free energy is given by^[7,8]

$$E_1^\pm = \frac{e}{C} \left\{ \frac{e}{2} \pm [ne - Q_p + (C_2 + C_g/2)V_a - C_g V_g] \right\} \quad (4)$$

$$E_2^\pm = \frac{e}{C} \left\{ \frac{e}{2} \pm [ne - Q_p - (C_1 + C_g/2)V_a - C_g V_g] \right\} \quad (5)$$

where Q_p can be considered as a polarization background charge induced by the gate field. The total capacity can be expressed as $C = C_1 + C_2 + C_g$. Obviously, free energy increment is affected by C , R , and the charge of the island.

2.3 Adopted method

Numerical simulation methods of SET mainly include the master equation and Monte Carlo^[6,7]. The master equation method is adopted in this paper due to its high precision. In order to acquire the state probability when the quantum dot is occupied by different numbers of electrons, the master equation is expressed as

$$\begin{aligned} \frac{\partial p(n,t)}{\partial t} = & [\dot{+}_1(n-1) + \dot{-}_2(n-1)] p(n-1) + \\ & [\dot{-}_1(n+1) + \dot{+}_2(n+1)] p(n+1) - \\ & [\dot{+}_1(n) + \dot{+}_2(n) + \dot{-}_1(n) + \dot{-}_2(n)] p(n) \end{aligned} \quad (6)$$

where n denotes the number of electrons within the island and p denotes the occupation probability. The current $I(t)$ can be expressed as $-e \dot{Q}(t)$. Because any occupation state contributes to the current, input current $I_1(V)$ and output current $I_2(V)$ are given by^[9,10]

$$I_1(V) = e \sum_{n=-\infty}^{\infty} p(n) [\dot{-}_1(n) - \dot{+}_1(n)] \quad (7)$$

$$I_2(V) = e \sum_{n=-\infty}^{\infty} p(n) [\dot{+}_2(n) - \dot{-}_2(n)] \quad (8)$$

In order to get steady solution, the left part of Eq. (6) is set to zero and the equation is simplified as

$$[\dot{+}_1(n) + \dot{+}_2(n)] p(n) - [\dot{-}_1(n+1) + \dot{-}_2(n+1)] p(n+1) = 0 \quad (9)$$

where $\dot{+}(n)$ is the sum of $\dot{+}_1(n)$ and $\dot{+}_2(n)$. $\dot{+}(n)$ denotes the increasing rate of electrons of the island while $\dot{-}(n)$ denotes the decreasing rate of electrons of the island. Figure 2 shows a flow chart of state probability according to Eq. (9).

3 Simulation results and analysis

Figure 3 is the I - V characteristics of the Al/

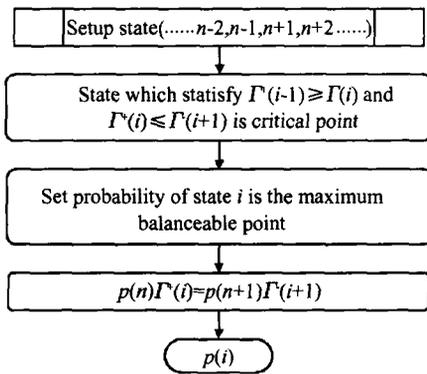


Fig. 2 Flow chart of state probability

AlO_x/Al SET which is manufactured by the so-called self-aligned in-line technique^[4] as reported by Bl ühner in 1997. The SET is composed by me-

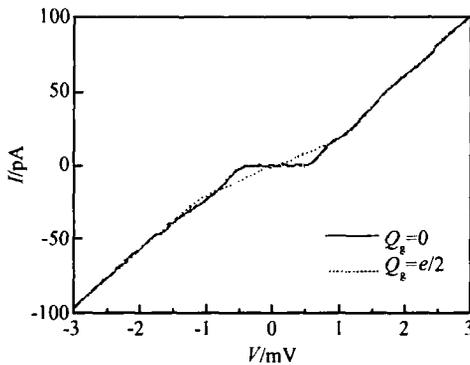


Fig. 3 I-V curves of the same Al/AIO_x/Al SET (T = 150mK)

tallic tunneling junctions ,so it can be numerically described by the model of this paper. In the report , the parameters are $C_g = (2.5 \pm 0.1) \times 10^{-17}$ F, $C = (2.7 \pm 0.3) \times 10^{-16}$ F, $C_1 = (1.7 \pm 0.2) \times 10^{-16}$ F, and $R = 10M$. Figure 4 shows the simulation results using the above parameters. There are obvious Coulomb blocks in both plots and the open voltages are the same when Q_g is zero. When Q_g is $e/2$,Coulomb block phenomenon will not happen. However ,their current values are different. From the simulated results ,it can be concluded that if the current values are also same ,resistance of a single tunneling junction will reach 12M . Because R of the tunneling junction in this experiment is estimated by asymptotes of the $I -V$ in the experiment ,it is not an accurate value.

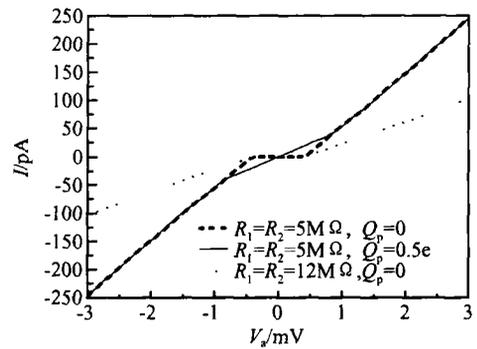


Fig. 4 Simulated I-V curves of the metallic tunneling junction SET (T = 150mK) with different resistances

Figures 5 and 7 show the $I-V_g$ curves and $I-V_a$ curves of a Nb/Nb oxide-based SET fabricated by utilizing a scanning probe microscope (SPM)-based anodic oxidation technique and thermal oxidation , as reported in 1997 by Shirakashi^[3] . The parameters are $C_1 = 0.08aF$, $C_2 = 0.05aF$, $C_g = 0.026aF$, $R_1 = 6.9 \times 10^{12}$, and $R_2 = 9.8 \times 10^{12}$. Importing these parameters into the model ,the simulated results are illustrated in Figs. 6 and 8.

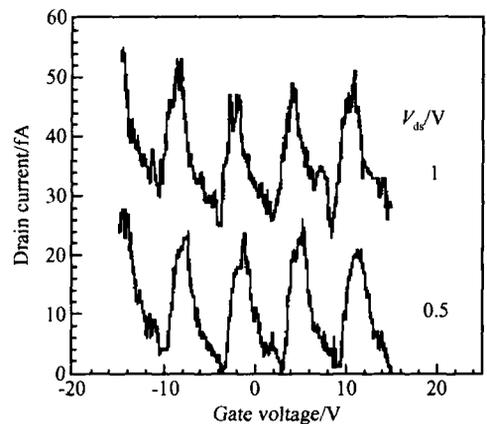


Fig. 5 I-V_g characteristics with several drain voltages at 298 K

The four plots can be divided into two groups , one composed of Fig. 5 and Fig. 6 and the other of Fig. 7 and Fig. 8. Comparing the two figures in each group ,it can be seen that the current values are different in simulated and experimental results ,although they do have the same trend. The parameters of the experiment are acquired using the Monte Carlo method and the time evolution of the

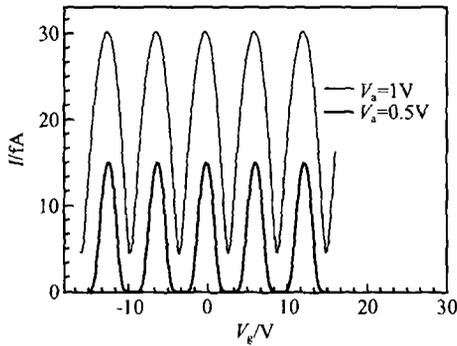


Fig. 6 Simulated $I-V_g$ characteristics with several drain voltages at 298 K

junction is calculated^[31]. In our model, if time evolution is considered, the occupation probability is different from that of the stationary case, which results in current discrepancy. Moreover, the current increases exponentially at higher drain voltage in Fig. 7, which is also due to the fact that the barrier suppression is caused by the image charge potential^[31], which is well known as the Schottky effect.

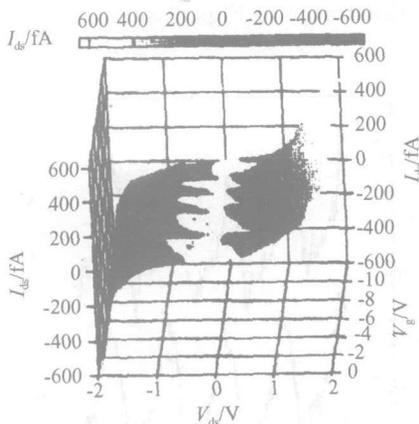


Fig. 7 $I-V_a$ characteristics with various side-gate voltages at 298 K.

Except for Fig. 8, the oscillation periods with the various gate voltages of the other three plots are the same, so the periods of the simulated results are correct. The reasons for the periods of figure different from the others still needs to be further investigated. On the other hand, the experimental curves are not as perfect as those of the simulation. Because the current value of SET is very small, feeble environment noise will greatly influence the result.

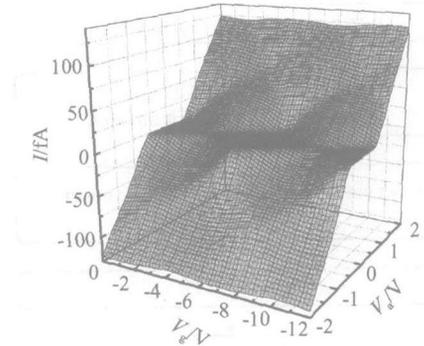


Fig. 8 Simulated $I-V_a$ characteristics with various side-gate voltages at 298 K

4 Conclusion

In this paper, the model of a single electron transistor of metallic tunneling junctions has been carried out using orthodox theory and the master equation method. In addition, the increment of free energy caused by electron tunneling is given in detail.

The shapes of simulated and experimental SET $I-V$ curves are similar, therefore the model is validated. Furthermore, for the same open voltages and the same periods of the $I-V_a$ curve in simulated and experimental results, the capacitance related parts in the SET model, such as C_1 , C_2 and C_g , are accurate. On the other hand, resistance related parts such as current values are different in simulated and experimental results. The reason which results in these differences is also discussed and the model must be improved further in the future.

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金属结单电子晶体管的模型建立及实验验证*

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摘要: 在正统理论的基础上,使用主方程法建立了金属结单电子晶体管的器件模型和算法流程. 将电容、电阻和温度等参数代入器件模型得到的 $I-V$ 特性曲线与实验结果吻合较好,从而验证了模型、算法以及程序流程的正确性. 此外,通过详细讨论模拟与实验的三组曲线差别,得到模型使用主方程的稳态解是导致模拟与实验之间结果存在差别的主要原因,即求解含时间的主方程将增加模拟精度;而且,指出镜像电荷引起的电势使电流随电压呈现指数增加的主要影响因素,明显偏离理论模拟的线性增加趋势.

关键词: 单电子晶体管; 正统理论; 库仑阻塞; 量子隧穿

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张立辉 女,1978年出生,硕士研究生,目前的研究方向是单电子晶体管的数值模拟.

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