# Charge Manipulations in Si-Based Quantum Dot Qubit Devices with Single Electron Transistors: Theory and Experiment

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## Abstract

A new model for calculations of the characteristics of the circuits with quantum dots and single-electron transistors is developed. The model takes into account the fact that the quantum dots in the circuit are not metallic for the purpose of determining the effective capacitance matrix in the circuit. The model is based on the solution of coupled Poisson and Schroedinger-like equations taking account of full 3D details of the real device. We demonstrate a very good agreement of the theory with experiment for many kinds of Si-based structures containing several single-electron transistors and isolated double quantum dots. The developed theory can therefore be used for design of the QD and SET circuits for quantum information processing.

#### 1. Introduction

Semiconductor structures with single electron transistors (SET) have been actively studied during last two decades [1,2]. Most recent applications of these devices are related to the quantum information processing, for example, when the isolated Si double quantum dot (QD) is used as a charge qubit and nearby SET is used as charge detector [3]. With increasing the number of active elements in the circuits (QDs and SETs) it is becoming very crucial to develop a theory that can predict the characteristics of the circuit from 3D geometry of the structure. In this paper we present such a theory and demonstrate that the relative change of the current can be predicted without any adjustable parameters when taking account of all details of the 3D structure design.

### 2. Theory and Results

We consider the Si-based structures with SETs (consisting of source, drain, gate and the QD) and, in some cases one or two Si isolated double QDs, the detailed description of the structure details and fabrication methods can be found in Refs. [4,5]. To model the circuit characteristics and, in particular, the relative change of the SET current in the regime of the charge detection, we have developed the theory that takes into account all important physical effects and the real 3D structure geometry. The modeling consists of the following stages:

(1) input the real structure from 2D SEM image of the real structure used in the experiment (see Fig. 1a);

(2) reconstruction of the 3D structure using the information about the layers thicknesses (Fig.1b);

(3) calculations of the effective capacitance matrix for the circuit by using 3D solution of the Poisson equation (see Fig.1c); in some cases (for smaller QDs) it is important to take account of the dimensional quantization in the QDs and solve coupled Poisson and Schroedinger equations. It is important to note, that unlike in the models with metallic QDs [6], for Si-based QDs the effective capacitance matrix is non-symmetric and could also contain negative effective capacitances.

(4) calculations of the SET currents through the solution of the master equations using the method described in [7] and the calculated effective capacitance matrix.

For capacitance calculations we solve the Poisson equation in 3D for a real device geometry; the boundary conditions on the QD interfaces are the same as for the dielectric interfaces. This is principally different from the case of metallic QD model [6], where the boundary condition as a constant potential on the QD interface is used. This means that in our model, the electric potential does vary inside the QDs and for the purpose of the capacitance matrix calculations we use the potential averaged over the QD volume (for some cases it is necessary to use as a weighting function for averaging the calculated electron wavefunction square modulus in the QD obtained from the solution of the Schroedinger equation). We found that this is principally important: using the "metallic" model the calculated SET characteristics (i.e. charging energy) differ from our model and the experiment by factor of 2-3, which proves that the QDs in circuits studied behave as semiconductor QD and not as a metallic island.

We demonstrate that the developed model can predict the SET characteristics (charging energy, period and asymmetry of the Coulomb diamonds) very well without any adjustable parameters, see Fig.1d,e. We also found that our model can describe the detection of the charge movements



Fig. 1 (a) Schematic view of the structure studied in Ref.[4] and the red dots showing the digitization of the 2D geometry of the structure for input into the model; (b) the 3D geometry of the structure created from 2D SEM image; (c) example of the electrical potential calculations in 3D; (d) Measured maps of the current  $|I_{QD1}|$  as a function of drain and top gate voltages (from Ref.4); (e) Calculated current map for same parameters as in (d); (f) Measured currents in the regime of charge detection; (g) calculated current in the regime of charge detection, same parameters as in (f).

in the circuit (see Fig.1f,g). When the electron is moving in/from one QD (QD1 in the example used in Fig.1), this results in sudden jump in the current of the nearby SET (see Fig.f,e). It is important to note that "metallic" model can not predict such detection correctly because the SET charging energy in this model is 2-3 times smaller than that in experiment.

## 3. Conclusions

We have developed the model that can predict the characteristics of the SET circuits without any fitting parameters, only using the detailed information about the 3D geometry as an input. The obtained results and the developed model can be therefore used as a tool to design Si-based circuits with isolated QDs and SETs for quantum information processing devices with one or several QD qubits.

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