Simulation study of charge modulation in coupled quantum dots in silicon

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1. Introduction
Electron spins are a promising candidate for solid-state quantum bits (qubits) [1]. In GaAs quantum dots (QDs), manipulation of electron spins have already been reported [2], however, the problem is a short decoherence time of electron spins due to hyperfine interaction. On the other hand, electron spins in Si are expected to have a long decoherence time owing to almost no nuclear spins. Since electrons in Si have a heavier effective mass compared to that of GaAs, the required size of Si-based QDs for spin qubit application should be much smaller than GaAs and hence there are only a few reports of the observation of Pauli spin blockade in Si double QDs (DQDs) without control of the number of charges [3, 4].

In order to manipulate electron spins in DQDs, it is preferable to reduce the number of electrons in each QD down to one, which can be detected by measuring charges using a charge sensor (CS) such as a single-electron transistor (SET) [5].

In this paper, we present simulation results of potential and electron concentrations in Si DQDs, in which the structure is the same as that we have observed Pauli spin blockade experimentally [3].

2. Device structure
The model structure we used for potential simulation is shown in Fig. 1(a). Si DQDs, an SET and side gates are fabricated by electron beam lithography and dry etching. The side gates are used for controlling potential of each QD and modifying tunnel rates through each potential barrier. Constricted regions controlled to be less than 10 nm width, by thermal oxidation after dry etching, make potential barrier for Si DQDs and an SET. Top gate deposited after thermal oxidation and CVD SiO2 formation is heavily doped poly-Si and used to induce 2-dimensional electron gas (2DEG) at the Si/SiO2 interface, like a gate of metal-oxide-semiconductor field-effect transistor (MOSFET) structure.

Figure 1(b) shows a top view SEM image of a device before deposition of the top gate. Si DQD and SET are schematically indicated by ovals. The thicknesses of a silicon-on-insulator (SOI) layer and buried-oxide (BOX) are 35 nm and 200 nm, respectively.

3. Result
We used ATLUS simulator from Silvaco Inc. for 3D potential simulation with various voltages applied to the top gate, SET bias, G1, G2 and G3 (Vtop, VSETbias, V G1, V G2 and V G3). With low voltages applied to the top gate, weak inversion layer is induced (Fig. 2 (a)). Therefore, the number of electrons in QDs can be modified easily by applying low voltage to V G1, V G2 and V G3 (Fig. 2 (b)). By means of integration of the electron concentration in QDs, we can deduce the number of electrons in each QD, which is one. In that case, however, contrast of electron concentration is low. It means electrons cannot be localized enough and a few-electron DQD is not formed by modifying each gate voltage.

When Vtop = 2 V, quantum confinement normal to the 2DEG becomes strong (Fig. 2 (c)). Furthermore, when VSETbias = -0.04 V and V G1 = V G2 = -2.4 V and V G3 = 0 V, small QDs are formed (Fig. 2 (d) and (e)). In this condition, electron concentration in DQDs is localized, and tunnel coupling between QDs remains slightly. An SET as a CS is essential to measure and control the charge states in DQDs.

4. Conclusions
We have investigated by simulation the potential and electron concentrations in Si DQDs with various applied voltages of the top gate and side gates. With top gate bias, the number of electrons can be controlled. With optimum side gates bias, electrons can be confined in QDs and coupling between QDs is controlled. With an SET as a CS, a few-electron condition can be monitored and hence makes spin manipulation possible.

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References
Fig. 1 (a) Model used for potential simulation. Si DQDs, SET and side gates (G1, G2 and G3) are covered by deposited SiO$_2$ and BOX. Top gate deposited after SiO$_2$ formation is shown as red transparent rectangular. (b) Scanning electron microscope (SEM) image of Si DQD device after etching of the SOI layer.

**Electron concentration distribution**

![Electron concentration distribution](image)

Fig. 2 (a-d) Electron concentration and (e) potential of the QDs with various voltages applied to top gate ($V_{\text{top}}$), SET bias ($V_{\text{SETbias}}$), and side gates G1, G2 and G3 ($V_{\text{G1}}$, $V_{\text{G2}}$ and $V_{\text{G3}}$). Top view and cross section of QDs are shown. The region of electron concentration less than $10^{14}$ cm$^3$ is ignored. Bias conditions: (a) $V_{\text{top}} = 1.0$ V and $V_{\text{G1}} = V_{\text{G2}} = V_{\text{G3}} = 0V$. Electron concentration in QDs is not high and the number of electrons is 8. (b) $V_{\text{top}} = 1.0V$, $V_{\text{G1}} = V_{\text{G3}} = -0.6V$ and $V_{\text{G2}} = 0V$. The number of electrons is 1, but the electron is not confined enough to form QDs. (c) $V_{\text{top}} = 2.0V$, $V_{\text{G1}} = V_{\text{G3}} = 0V$ and $V_{\text{G2}} = 0V$. Electron concentration in QDs is high and the number of electrons is 12. (d) $V_{\text{top}} = 2.0V$, $V_{\text{G1}} = V_{\text{G3}} = -2.4V$, $V_{\text{G2}} = 0V$ and $V_{\text{SETbias}} = -0.04V$. The number of electrons is 2, and the electrons are confined to form QDs. Inset: Zoom of inter-QD coupling region with the corresponding color scale bar. A small region with electron concentrations of higher than $1x10^{14}$ cm$^3$ contributes for tunnel coupling between QDs. (e) Potential distribution for the condition shown in (d). Inset: Zoom of QDs. Potential barrier of source/drain constriction is higher than that of inter-QD coupling.