Detection of Quantum Cellular Automaton Action in Silicon-on-insulator Cells

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Detection of Quantum Cellular Automaton Action in Silicon-on-insulator Cells

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We present a proposal for an experiment to demonstrate QCA (Quantum Cellular Automaton) functionality for a cell fabricated with silicon-on-insulator technology. The fundamental feature of a working QCA cell consists in the anticorrelated transition of electrons in the two pairs of dots forming the cell: we show how such a phenomenon can be detected from the appearance of a "locking" effect between the Coulomb Blockade current peaks relative to each pair. The proposed approach allows the detection of QCA action without the need for additional noninvasive charge detectors probing each dot. We have performed detailed numerical simulations on the basis of interdot capacitance values obtained from experimental data and determined the range of parameters within which the effect should be detectable.

Keywords: Quantum Cellular Automata; Silicon; Monte Carlo

1. INTRODUCTION

The Quantum Cellular Automaton concept, first proposed by Lent *et al.* [1], is an interesting approach to nanoelectronics, based on two-dimensional arrays of bistable cells, which allow the implementation of arbitrary combinatorial logic circuits. The basic cell is made up of four quantum dots and contains two electrons: if confinement in each dot is strong enough, the electrons will repel each other, and will tend to align along one of the diagonals of the square cell. In the absence of external electric fields or of other nearby cells, alignment along either diagonal is equally probable. If we place, next to the cell we are considering, another cell with a well defined polarization (indicated as "driver cell" in the following), the electrons in the "driven cell" will tend to align parallel to those in the driver cell. If a logic value is associated with each polarization configuration, it is apparent that such a value can be propagated along a line of cells (binary wire) in a domino-like fashion and it has been shown that combinatorial logic functions can be easily obtained [2] by properly assembling two-dimensional arrays of cells. This approach would have the advantage of very limited power dissipation, since charges move only within a cell and there is no net charge flow across the array, and significant perspectives for extreme miniaturization, down to the

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molecular level. However, many complex technical problems need to be solved before this technology can be applied to practical purposes; in particular viable solutions must be found to the issues of fabrication tolerances [3] and of detecting the occupancy of each dot without perturbing the cell state.

The first experimental demonstration of a QCA cell was obtained [4, 5] with metallic tunnel junctions with $Al/AlO_x/Al$ tunnel barriers, with a setup in which electrons are supplied to the cell *via* external leads and polarization was measured by means of charge amplifiers based on single-electrons transistors capacitively coupled to the metal islands.

A different approach is represented by the fabrication of a 4-dot cell with GaAs/AlGaAs technology, defining the dots by means of properly shaped metal gates, deposited on top of a heterostructure. In this case it is possible to fabricate minimally invasive charge detectors by means of quantum point contacts, whose resistance is influenced by the charge stored in the quantum dots.

The QCA cell implementation on which we are currently focusing is based on silicon dots [6] defined by electron beam lithography and successive size reduction by means of controlled oxidation on silicon-on-insulator material. This approach has the advantage of allowing the fabrication of extremely small dots (in the 10 nm range) and of improving the strength of the electrostatic interaction in comparison to materials such as GaAs, due to the reduced dielectric permittivity of silicon oxide. It would be possible to add also charge detectors, in the form, for example, of single-electron transistors, but this would translate into added complexity for a structure that already requires extremely challenging tuning procedures to obtain simultaneous operation of the four dots.

We propose a measurement procedure that can provide a clear demonstration of correlated electron switching between the two pairs of quantum dots forming a cell from the observation of the relationship between the position of the Coulomb Blockade current peaks through the dot pairs. A Monte Carlo code has been developed for the validation of the proposed procedure and the determination of the appropriate parameter values.

2. PRINCIPLE OF OPERATION

The proposed experiment will be described with reference to the layout represented in Figure 1, corresponding to the structure fabricated by Single *et al.* [6] in silicon-on-insulator material. There are four lithographically defined islands, with four adjustment gates. The barriers separating the dots belonging to the same pair and those separating the dots from the leads are obtained as geometrical constrictions. Such a device can be represented, for the sake of investigating its electrical behavior, with the equivalent circuit of Figure 2, where the T_E's and T_D's are tunneling capacitors. In this cell, tunneling can occur only between dots belonging to the same pair, contrary to "classical" QCA cells, in which all dots are connected *via* tunneling barriers. This does not represent a significant

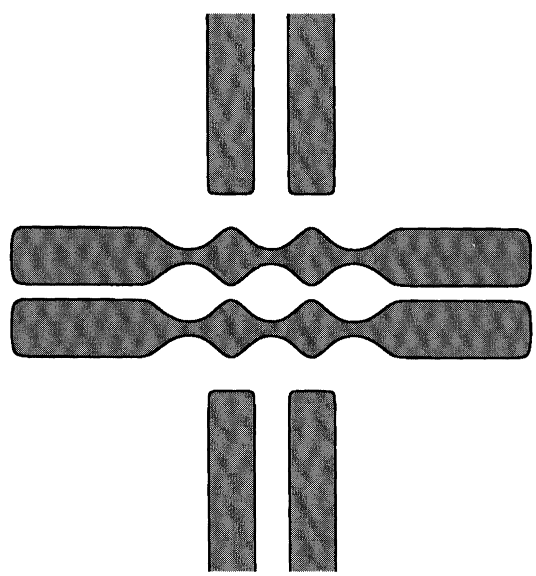

FIGURE 1 Sketch of the Si-SiO_2 QCA cell. Oxidized silicon is represented in grey. Tunnel capacitances correspond to the six constrictions.

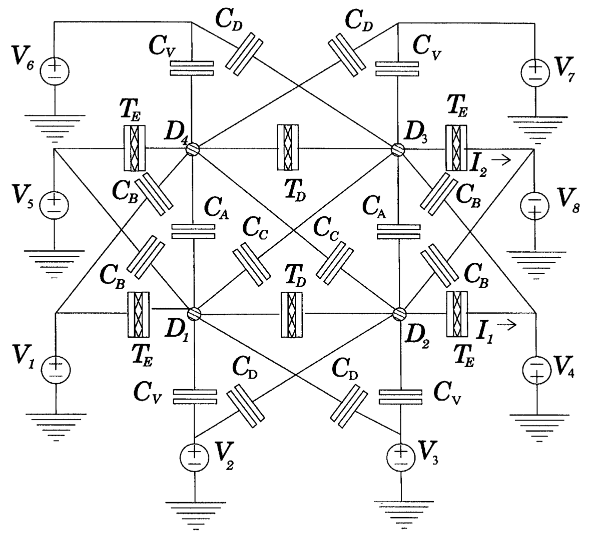

FIGURE 2 Equivalent capacitance network of the QCA cell.

difference from the operational point of view, since charge configurations are the very same in both cases. In Figure 2 we did not include the capacitances between the adjustment leads and the diagonally opposite dots, for the sake of simplicity. We have included them in our calculations and noticed no relevant contribution. The same can be said for the capacitances between the dots and the backgate that is usually present under the structure.

In order to understand the proposed procedure, it is convenient to focus first on the operation of a single pair of dots, considering all voltage sources connected to the other pair of dots as deactivated and the corresponding electrodes as grounded. In the presence of a small voltage applied between the left and right lead, a current will flow through the three tunneling junctions in a dot pair only if the chemical potentials of the three dots are aligned with those of the leads, which corresponds to having both dots on the edge between two stable occupancies.

The chemical potentials in the dots can be varied by means of the voltage applied to the adjustment gates: if we apply a positive voltage ramp to the gate controlling the left dot and a negative ramp to that connected to the right dot, and adjust the relative position of the ramps in such a way as to synchronize the transition from $M+1$ to M electrons in the right dot with that from $N-1$ to N in the left dot, the Coulomb Blockade will be lifted and a current peak will be observed through the dots. The same will happen in correspondence with any other synchronous change of the occupancy in the two dots. We assume that the rate of variation for the applied voltages is very slow compared to the tunneling rates and to the RC time constants, so that a quasi-static treatment is in order.

The experiment can then be repeated for the upper pair of dots (grounding the voltage source connected to the lower pair), applying a ramp with positive slope to the adjustment gate for the right dot and a ramp with negative slope to the other gate, in order to obtain transitions in dot occupancy that are opposite to those achieved in the lower pair of dots. A shift is also included with respect to the ramps for the lower pair, in order to displace the peaks of I_2 with respect to those of I_1, as shown in Figure 3.

If both the upper and lower section are operated simultaneously, the electrostatic interaction between the dots will determine a synchronization between opposite occupancy variation phenomena, thereby yielding a "locking" effect between the peaks in the two currents (see Fig. 4), despite the presence of the above mentioned shift.

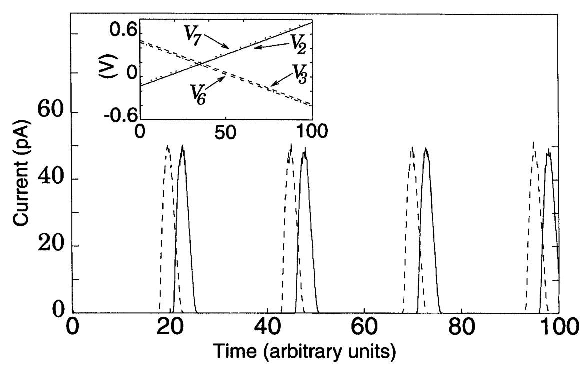

FIGURE 3 Time dependent current through the upper dots (solid line) and through the bottom dots (dashed line) when the other semicell is switched off.

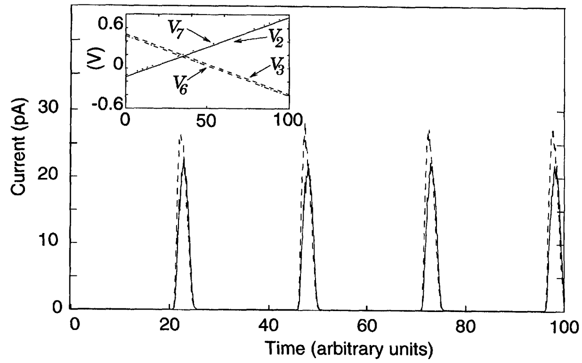

FIGURE 4 Time dependent current through the upper dots (solid line) and through the bottom dots (dashed line) when both semicells are biased. The synchronization of current peaks implies QCA operation.

This will demonstrate correlated switching and, therefore, cell operation.

3. SIMULATION CODE

Our initial checks on the feasibility of the proposed experiment were performed with the public domain version of the well-known SIMON [7] single electron circuit simulator, but we then developed our specifically devised Monte Carlo simulator in order to obtain a better numerical precision and a more direct control of internal parameters. The computational strategy is quite straightforward and analogous to what has appeared in the literature for single electron circuits.

The simulation is subdivided into a number of steps, each corresponding to a given value of the gate voltages. Within each step a stationary Monte Carlo calculation is performed, letting the electrons cross the tunneling junctions according to the following rules: the variation of free energy ΔE associated with the crossing of each junction is computed, then the tunneling rates are evaluated according to the "orthodox" Coulomb blockade theory:

$$\Gamma = \frac{1}{e^2 R_T} \frac{\Delta E}{1 - \mathrm{e}^{-\Delta E/(k_B T)}},$$

where R_T is the tunneling resistance, e is the electron charge, k_B the Boltzmann constant and T the temperature. A random number is generated, uniformly distributed in an interval which is partitioned into sections with a width proportional to the rate for each possible transition: the transition corresponding to the section containing the generated random number is then chosen. Dot charges are updated as a result of the transition and a new iteration is performed, after generating the time elapsed during the current iteration as an exponentially distributed random number with average equal to the inverse of the total tunneling rate (obtained as the sum of the rates for all possible transitions). The procedure is repeated a number of times sufficient to get reliable estimators of the quantities of interest: the charge in each dot, obtained by averaging the values at each iteration, and the current flowing through each junction, determined by taking the ratio of the total charge that has traversed it to the sum of the times corresponding to each iteration.

The whole sequence is repeated for all the gate voltage values into which the simulation has been subdivided and results for the dot charges and junction currents are collected. Our code has been tested on the structures of Ref. [6], and has yielded results that are in extremely good agreement with the experimental data.

4. NUMERICAL RESULTS AND FEASIBILITY ASSESSMENT

The values of the geometrical capacitances between dots have been evaluated by means of the FASTCAP [8] program, modeling the various electrodes as parallelepipeds approximating the actual geometries. We have assumed a dot size of $60 \times 60 \times 60\,\mathrm{nm}$, and a separation of $16\,\mathrm{nm}$ between dots and of $100\,\mathrm{nm}$ between each dot and the corresponding adjustment gate. Separation between dots belonging to different pairs must be very small, otherwise coupling is too weak to allow proper operation. As a rule of thumb, we have found out that values of the coupling capacitances between the upper and lower dots must be of the same order of magnitude as that of the tunneling junctions. With this procedure the following results have been obtained: $C_D = 0.94\,\text{aF}$, $C_V = 1.65\,\text{aF}$, $C_B = 1.36\,\text{aF}$, $C_C = 1.0\,\text{aF}$, $C_A = 0.94\,\text{aF}$. The capacitances of the tunnel junctions cannot be computed from simple geometrical considerations, since, as it turns out from the experiments, localization in the dots and creation of the barriers between them is substantially the consequence of the potential fluctuations due to the random distribution of dopants. We have therefore resorted to recent measurement results [6] yielding the values: $T_E = 9\,\text{aF}$ and $T_D = 10\,\text{aF}$.

As a consequence of their relatively large value, operation is possible only at very low temperatures, in order to avoid excessive thermal broadening that would prevent observation of the "locking" effect. We have performed calculations for a temperature of 0.2 K, with external bias voltages $V_1 = V_4 = V_5 = V_8 = 1.7\,\text{mV}$.

We start with V_5, V_6, V_7, V_8 turned off, *i.e.*, with the upper part of the cell disabled, and apply the previously described voltage ramps to the adjustment gates. The resulting current I_1 flowing through the lower dots is reported in Figure 3 with a dashed line. The time evolution of the adjustment voltages is reported in the inset. The whole procedure is then repeated for the upper section, disabling the lower section. The voltage sources connected to V_6 and V_7 deliver voltage ramps corresponding to those previously supplied by V_3 and V_2, respectively , but with a 7 mV shift, which determines a displacement of the curve for I_2 (reported with a solid line in Fig. 3) with respect to that for I_1.

The final phase consists in operating both the upper and lower section of the cell at the same time: the peaks in I_1 and I_2 are now locked, as shown in Figure 4, which represents evidence of the correlated switching between the two halves of the cell and therefore of QCA action. The locking effect is very sensitive to the choice of parameters, in particular to the already mentioned coupling capacitances between the upper and lower dots, and to the temperature. If the coupling capacitances are reduced by a factor 10, no locking occurs, due to the insufficient electrostatic interaction between the upper and lower halves. Operation with the considered layout is disrupted also if temperature is increased above about 1 K, due to thermal broadening of the current peaks, and the ensuing impossibility to distinguish the actual separation between the peaks for I_2 and I_1, unless this is so wide that locking cannot take place even with relatively large coupling capacitances.

5. CONCLUSIONS

We have proposed an experiment for the demonstration of QCA action with silicon-on-insulator technology, based on the detection of the electrostatic interaction between the two halves of a cell made up of four silicon quantum dots embedded in silicon oxide. A numerical Monte Carlo simulator has been devised, which has allowed the determination of the range of circuit parameters suitable for the experimental observation of correlated switching between the two cell halves. The major difficulties, from the point of view of the actual experimental implementation, consist in obtaining large enough coupling capacitances between the upper and lower dots and in performing measurements at temperatures below 1 K, with the associated decrease in current levels, due to the reduced number of carriers. Overall, however, the experiment appears to be feasible, and its implementation is currently being pursued.

Acknowledgments

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