Simulation of a non-invasive charge detector for quantum cellular automata

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G. Iannaccone, C. Ungarelli, M. Macucci, E. Amirante, M. Governale, *Simulation of a single charge detector for quantum cellular automata*", Thin Solid Films, **336**, pp.145-148 (1998).

Thin Solid Films 336 (1998) 145–148

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Abstract

Information in a quantum cellular automata architecture is encoded in the polarization state of a cell, i.e. in the occupation numbers of the quantum dots of which the cell is made up. Non-invasive charge detectors of single electrons in a quantum dot are therefore needed, and recent experiments have shown that a quantum constriction electrostatically coupled to the quantum dot may be a viable solution. We have performed a numerical simulation of a system made of a quantum dot and a nearby quantum point contact defined, by means of depleting metal gates, in a two-dimensional electron gas at a GaAs/AlGaAs heterointerface. We have computed the occupancy of each dot and the resistance of the quantum wire as a function of the voltage applied to the plunger gate, and have derived design criteria for achieving optimal sensitivity.

Keywords: Non-invasive charge detector; Quantum cellular automata

1. Introduction

Logic circuits based on the quantum cellular automata (QCA) paradigm offer an interesting alternative to traditional architectures used for computation [1,2]. The basic building block of a QCA system is a cell made up of four or five quantum dots, and containing two electrons, which can align along one of the two diagonals, giving rise to two possible polarization states. It has been shown that cell polarization can propagate along a chain of cells and that properly assembled two-dimensional arrays of cells allow the implementation of logic functions. The results of any computation performed with such arrays consist in the polarization state of some output cells. This information must be read without perturbing it, therefore a non-invasive charge probe is needed.

Recent experiments have shown that it is possible to detect a single electron being added to a quantum dot by measuring the resistance of a quantum point contact placed next to it [3]. The electrostatic potential defining the constriction is modified by the contribution of the additional electron, so that the transmission coefficients and, consequently, the overall resistance are affected.

We have performed a numerical simulation of a system made of a quantum dot and a nearby quantum point contact defined, by means of depleting metal gates, in a two-dimensional electron gas at a GaAs/AlGaAs heterointerface. The occupancy of each dot and the conductance of the quantum wire are calculated as a function of the voltage applied to the plunger gate for a few initial wire resistances. The details of the simulations are described in Section 2, while the results are discussed in Section 3.

We show that the highest sensitivity for charge detection is obtained for bias voltages such that the initial resistance of the quantum wire is rather high, of the order of 100 kΩ, when conduction through the quantum wire is substantially in the tunneling regime, so that even extremely small variations of the confinement potential (such as those due to the addition or removal of a single electron) produce measurable variations of the resistance.

2. Simulation

The system we focus on is realized on the heterostructure sketched in Fig. 1, consisting of an undoped GaAs substrate, an undoped 20-nm thick $Al_{0.36}Ga_{0.64}As$ spacer layer, a silicon delta doping layer of 6×10^{12} cm^{-2}, an undoped 10-nm thick $Al_{0.36}Ga_{0.64}As$ layer, an undoped 5-nm thick GaAs cap layer. An unintentional acceptor doping of 10^{15} cm^{-3} is considered in all undoped layers, while the delta doping is modeled as a uniform doping on a 10-nm layer.

The gate configuration is shown in Fig. 2: the quantum

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PII S0040-6090(98)01316-9

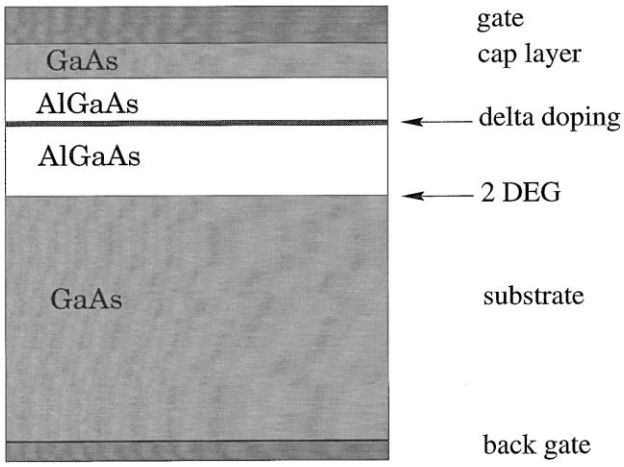

Fig. 1. Layer structure consisting of a GaAs substrate, 20 nm undoped AlGaAs spacer, Si delta doping layer (6×10^{12} cm^{-2}), 10 nm undoped A1GaAs, 5 nm GaAs cap layer.

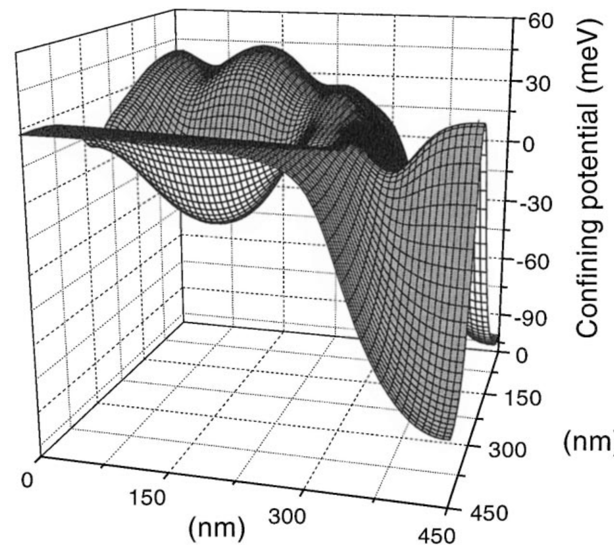

Fig. 3. Confining potential for the electrons in the plane of the GaAs–A1GaAs heterointerface.

dot is defined by gates 1, 2, 3 and 4, and has a geometrical area of 188×104 nm; the detector is the constriction between gates 4 and 5. The bias voltage V_i of gates i ($i = 1, \ldots, 4$) is -0.12 V, while we have considered a few different voltages V_5 for gate 5, between -0.15 and -0.9 V, corresponding to different initial resistances of the quantum costriction (from 7.6 kΩ to 520 MΩ).

A detailed simulation of the system would require the self-consistent solution of the Schrödinger and Poisson equations on a three-dimensional grid, in order to obtain the conduction band edge and the electron density profiles in the simulation domain. Then, the resistance of the quantum point contact could be evaluated by means of the recursive Green's function formalism, [4] using the potential landscape obtained from the Poisson–Schrödinger solver, while the charge contained in the quantum dot could be simply obtained by integrating the electron density in the dot region. In order to assess the functionality of the detector, the voltage of the plunger gate must be swept towards more negative values, as to progressively deplete the quantum dot, and the induced quantum wire resistance must be calculated. The simulation sketched above should be therefore repeated a large number of times, and would be prohibitively time consuming.

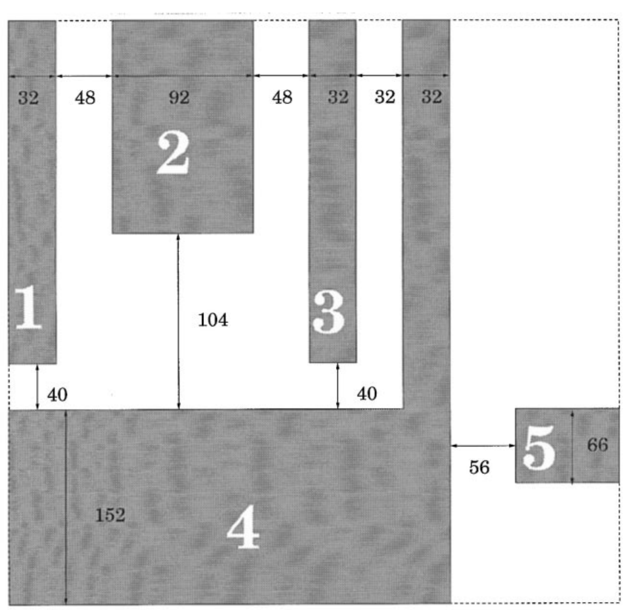

Fig. 2. Gate configuration defining the quantum dot and the detector (dimensions are in nanometers). Gate 2 is the plunger gate; the voltage applied to gate 5 modulates the resistance of the detector.

For this reason, we have chosen a less rigorous approach, which is, however, much simpler from the computational point of view. First, the Poisson equation is solved on a 3D grid ($65 \times 65 \times 65$ points) with a semiclassical approximation: the electron and hole densities are determined from the density of states in the bulk and the Fermi–Dirac distribution, while acceptors are considered fully ionized. Dirichlet boundary conditions are enforced for the potential at the gate surfaces, while Neumann boundary conditions are enforced at the exposed GaAs surface, with a normal component of the field equal to 88.2 V/μm, i.e. the value computed with all the gates at 0 V. The Fermi level at equilibrium is pinned 5.25 eV below the vacuum level, which is the value that provides the best fit of the pinch-off voltage with experiments (Y. Jin, pers. commun.). On the lateral boundary regions of the simulation domain, Neumann boundary conditions with zero electric field are enforced.

The contribution to the potential from the charge in the dot is calculated by solving again the Poisson equation, using the charge in the dot as the only source term, and is subtracted from the previously calculated potential, in order to obtain the confining potential for the electrons.

At this point the 3D problem is decoupled into a 2D

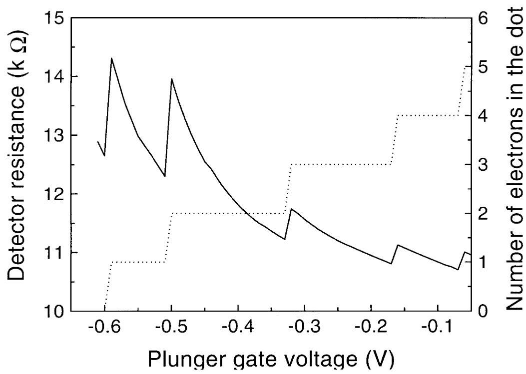

Fig. 4. Detector resistance (solid line) and number of electrons in the dot (dashed line) as a function of the voltage applied to the plunger.

problem at the heterointerface plane, and a 1D problem in the vertical direction, under the assumption that confinement in the vertical direction is much stronger than that on the horizontal plane. The one-dimensional Schrödinger equation is solved in the vertical direction, and the energy of the first subband is obtained with respect to the conduction band bottom in GaAs at the heterointerface: by adding this value to the conduction band edge of the heterointerface plane, we obtain the confining potential for electrons in the 2DEG, which is reported in Fig. 3 for the case of $V_5 = -0.16$ V.

A 2D Schrödinger–Poisson self-consistent solver is used to determine the dot occupancy and the charge distribution [5]. The electron–electron interaction is modeled consistently with the Neumann conditions enforced at the exposed surface, i.e. with negative image charges. Finally, the confining potential in the quantum wire is calculated by adding to the previously obtained confining potential the contribution of the electron density in the dot computed with the Schrödinger–Poisson solver.

When the plunger gate voltage is modified, instead of solving again the 3D Poisson equation, we use a semi-analytical method [6] to evaluate the correction to the confining potential on the plane of the 2DEG, assuming that the other charges in the structure remain unchanged.

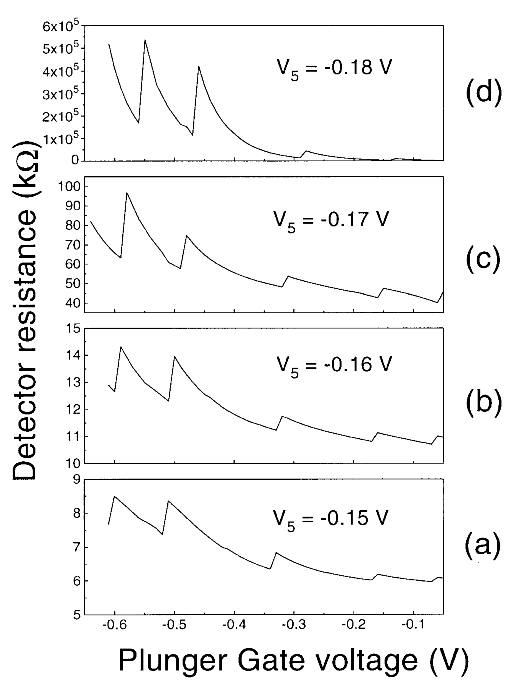

Fig. 5. Detector resistances as a function of the voltage applied to the plunger gate for four different values of the voltage V_5. For V_5 lower the -0.18 V the quantum wire has negligible conductance.

3. Results and discussion

In Fig. 4 the results of the simulation for $V_5 = -0.16$ V are shown: for a plunger gate voltage V_2 of -0.61 V the dot is completely depleted and the detector resistance is 12.9 kΩ. As V_2 is raised in steps of 10 mV the confining potential on the heterointerface plane is lowered, therefore the number of electrons in the dot N (dashed line) progressively increases.

The detector resistance decreases for increasing plunger gate voltage as long as N is constant. Instead, when one electron is added to the dot, Coulomb repulsion raises the confining potential of the quantum costriction, causing an increase of a few percent of the detector resistance.

We have also studied the dependence of the detector sensitivity upon the initial resistance of the quantum constriction. In Fig. 5 the detector resistance is plotted as a function of the plunger gate voltage for four different voltages applied to gate 5, ranging from -0.15 to -0.18 V: of course, the lower the voltage applied to gate 5, the higher the initial detector resistance. As can be seen, a high sensitivity can be obtained if conduction in the quantum wire is essentially in the tunneling regime, as in the cases of Fig. 5d,c, corresponding to an initial resistance much higher than that associated with a single propagating mode in the quantum wire (i.e. 12.728 kΩ). This is simply due to the fact that the transmission probability in the case of tunneling is extremely sensitive to a variation of the confining potential profile. For values of V_5 lower than -0.18 V the quantum wire is practically pinched off.

In order to have a detectable current through the detector in quasi-equilibrium condition, an initial resistance close to 100 kΩ, as in the case of Fig. 5c, seems the better solution, since it also provides a relative change in the detector resistance larger than 10% when one electron is added.

In conclusion, the electrostatic coupling between the dot and the constriction seems to be a viable detection principle for quantum cellular automata systems. A more complete simulation, including the four dots and the associated detectors, would be useful to really verify whether the ‘stray’ capacitive couplings between a detector and the other dots can undermine correct detection.

Acknowledgements

This work has been supported by the ESPRIT Project 23362 QUADRANT (Quantum Devices for Advanced Nano-Electronic Technology). The authors wish to thank J. Martorell for making available the code implementing the method of Davies et al. [6].

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