*VLSI DESIGN*
2001, Vol. 13, Nos. 1–4, pp. 149–153
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# Simulation of a Complete Chain of QCA Cells with Realistic Potentials

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We present a numerical simulation of the operation of a chain of 3 Quantum Cellular Automanton (QCA) cells, with the inclusion of a realistic procedure to enforce, with an externally applied bias voltage unbalance, the polarization of the first cell. The polarization state is shown to propagate correctly, as long as the bias unbalance applied to the electrodes of the first cell is not so large as to directly perturb nearby cells. The addition of dummy cells is needed to balance the asymmetries existing at the ends of a chain: this is an indication of further difficulties, that may become relevant if fabrication of more complex arrays is attempted.

*Keywords*: Quantum cellular automata; Bistability; Quantum dots

## 1. INTRODUCTION

The concept of QCA (Quantum Cellular Automaton) logic was proposed by Lent *et al.* [1] in 1993, as an alternative approach to nanoelectronic digital circuits. In the last few years detailed modeling of QCA cells with realistic potentials has uncovered serious problems with geometrical fabrication tolerances, while other issues, such as the enforcement of the polarization state of the input cell and its propagation along a chain of cells, have been intensely debated, but no simulation for a well-defined and realistic layout for any semiconductor-based implementation has actually been performed. We present an extension of our QCA cell simulator based on the Configuration-Interaction technique to a layout with three cells, in which the first cell is controlled adjusting the voltages applied to the gates defining it.

If we consider a cell layout based on independent gates [2], the polarization of the driver cell can be easily obtained by creating a very small electrical asymmetry among the electrodes.

We consider a GaAs/AlGaAs heterostructure, with a 2DEG (2-dimensional electron gas) at 35 nm from the surface and compute the confining potential at the 2DEG level with the semianalytical method due to Davies *et al.* [3], including also the effect of image charges, associated with the assumption of Dirichlet boundary conditions at the surface [4]. The presence of the electrodes

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defining a neighboring driver cell would create a perturbation sufficient to completely alter the symmetry of the driven cell: their action must be balanced by another, symmetrically placed cell. In turn, to balance the driver cell, we need to add more cells on the sides, symmetrically with respect to it.

Our goal is to demonstrate that enforcing the polarization of a driver cell requires a very small bias change, which does not affect significantly the nearby cells, and therefore allows a correct propagation of the polarization state: a small change in the electrostatic potential triggers a rearrangement of the cell charges, which produces a much larger and opposite variation of the overall potential felt by the adjacent cell, thereby leading to its appropriate polarization.

## 2. MODEL

In previous work on the simulation of QCA cells with realistic potentials, we always studied the response of a single driven cell to the action of a driver cell, whose polarization was assumed as defined *a priori*. In a real chain of cells, the polarization of the driver cell has to be enforced with some technique that must not perturb significantly the electrostatic potential in the nearby cells, and, for each cell, we must take into account the electrostatic action from all the other cells and the electrodes defining them.

We assume a depth of 35 nm from the surface for the 2DEG (2-dimensional electron gas) and compute the confining potential at the 2DEG level with the semianalytical method due to Davies *et al.* [3], which allows the determination of the potential $V_g(x, y, z)$ produced by an arbitrary polygonal gate on top of a heterostructure:

$$V_g(x,y,z) = \frac{1}{2\pi} \int_S \frac{|z| V_g(x', y', 0)}{(x-x')^2 + (y-y')^2 + z^2}. \quad (1)$$

In order to have a reliable estimate of the range of gate potential values that can be applied while still obtaining properly formed quantum dots, we include in our calculations of the potential at the 2DEG level the constant term deriving from the Fermi level pinning, the surface charge and the layer doping. Such a constant term is estimated as indicated in Ref. [5], considering a standard GaAs/AlGaAs heterostructure with a 10 nm GaAs cap layer, a 15 nm AlGaAs doped layer, a 10 nm AlGaAs spacer layer and a GaAs substrate. The Fermi level at the surface is assumed to be pinned at 0.65 eV from the conduction band, we consider a surface charge density of $5 \times 10^{12}$ electrons/cm$^2$ and a doping of $3.71 \times 10^{18}$ cm$^{-3}$. The separation between the centers of adjacent cells has been assumed to be 326 nm.

The overall confinement potential, obtained from Eq. (1) and the estimate of the constant term, lies under the Fermi level in small regions where the quantum dots form. The presence of the electrodes defining a neighboring driver cell would create a perturbation sufficient to completely alter the symmetry of the driven cell: their action must be balanced by another, symmetrically placed, cell. In turn, to balance the driver cell, we need to add more than one cell, we must add a large enough number of cells on both sides, so that each cell can see the same gate arrangement in both directions, at least as far as the distance where the electrostatic interaction has practically vanished. Increasing the intercell spacing is not an option, because this would reduce the already small energy splitting between the correct and the incorrect electron configuration [6]. We have determined that, to study 3 coupled cells, a chain of at least 11 cells is needed; we used 21 cells in our calculations to make sure that there are no undesired asymmetry effects. Only the three central cells are active, while the others are dummy, in the sense that only the action of their gates is considered, not that of their electrons. The influence of such electrons on the polarization state of the three active cells is negligible, as in general the "feedback" effect of driven cells (evidence for this conclusion will be provided in the following by the fact that self-consistence is reached with

just one iteration). As already discussed in Ref. [2], a QCA cell can be defined by means of seven independent depletion gates, as shown in Figure 1; this allows us to obtain a perturbation in the potential and consequently the enforcement of a given polarization for the driver cell by simply adjusting the gate voltages. In particular, with reference to the numbering in Figure 1, the driver cell polarization is obtained by slightly raising the modulus of the voltage applied to electrodes 3 and 7. This causes a progressive depletion of the lower left and upper right dots and induces electron localization in the upper left and lower right dots.

To limit the complexity of our calculations, an occupancy of only two electrons per cell has been assumed. It has however been demonstrated [7] that proper operation of QCA cells is possible whenever the number of electrons equals $4N+2$, where $N$ is an arbitrary integer. Most properties of QCA cells are not significantly affected by the addition of a multiple of 4 electrons, therefore results obtained for 2-electron cells can be extrapolated to generic cells with $4N+2$ electrons.

The bias voltage for electrodes 1, 3, 4, 5, 7 is set at $-0.8$ V, and that for gates 2 and 6 at $-0.9$ V. The resulting confinement potential at a depth of 35 nm is shown in Figure 2 for a three cell

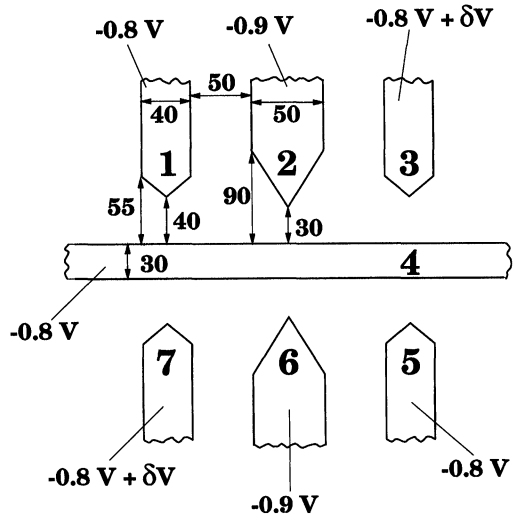


FIGURE 1 Gate layout defining the driver cell (all measurements are expressed in nanometers).

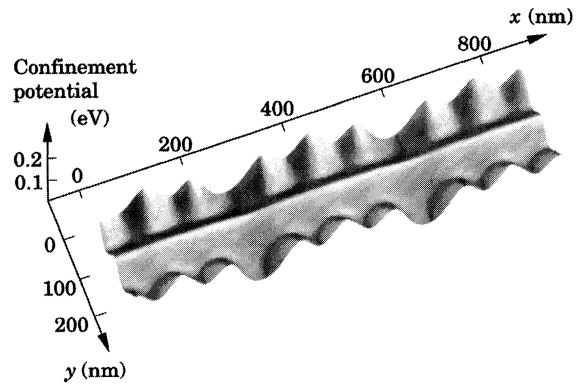


FIGURE 2 Electrostatic potential at the 2DEG depth for a three-cell sequence.

sequence: four potential minima are visible in correspondence with each cell. Since with these feature sizes operation is possible only at temperatures below 100 mK, we perform all calculations at zero temperature.

We use the Configuration Interaction (CI) method [2], which is based on the representation of the many-electron wave function with a linear combination of Slater determinants. Once the confinement potential has been obtained with the above mentioned semianalytical procedure, the electron density in the driver cell is computed with the CI method, using a basis of 28 Slater determinants. Then the electron density in the first driven cell is determined, considering the electrostatic potential due to the gates and the action of the charge distribution in the driver cell. Analogously, the electron density in the second driven cell is computed including the effects of the gates and of the charge distributions in the two other cells. Finally, the calculation is repeated for each cell, considering all contributions, until convergence is reached, *i.e.*, until the electron densities at two consecutive iterations for each cell differ less than a threshold value.

## 3. NUMERICAL RESULTS

In a realistic chain, enforcing the polarization of the driver cell represents an issue that needs to be

dealt with very carefully: due to the extreme sensitivity of the system, even a vanishingly small gate voltage perturbation can be expected to lead to a significant variation in the electron distribution, and, possibly, to undesired effects on the nearby cells. Different values of the voltage shift $\delta V$ between the electrodes defining the first (driver) cell of the sequence have been investigated, and the charge rearrangement within the cell has been calculated.

A $\delta V$ term was added to the potential of gates 3 and 7. It has been found that a value of $\delta V = -10^{-6}$ V is sufficient to force the two electrons into the dots closer to gates 1 and 5, therefore, according to the polarization expression of Ref. [1], the polarization state of the driver cell is $P_{driver} = -1$. Such a charge rearrangement determines a polarizing field that is sufficient to fully bias the neighboring cell (first driven), which, in turn, causes the polarization of the third cell.

In Figure 3 we report the electron density in the three cells, when a perturbation of $-10^{-6}$ V is applied to the driver cell: proper propagation of the polarization is obtained. It is important to note that the effect of the voltage shift applied to gates 3 and 7 of the first (driver) cell on the second (first driven) and third (second driven) cell is opposite to that exerted on the local electron configuration of the driver cell itself. Therefore, such a voltage shift would tend to cause a charge distribution in the driven cells corresponding to $P_{driven} = 1$. This effect is however completely overwhelmed by the electrostatic action of the two electrons in the driver cell, so that correct polarization propagation occurs.

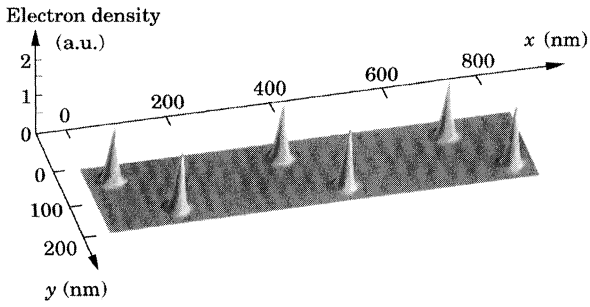


FIGURE 3 Electron density in a chain of three cells when the polarization state of the first cell is enforced by applying the appropriate gate voltage unbalance.

The situation changes if we increase the magnitude of the voltage shift applied to the electrodes of the driver cell. We have found a threshold value, for the specific layout we are discussing, at $|\delta V| = 0.6$ mV: when the perturbation becomes greater than this threshold, the electrostatic action from the electrons in the driver cell is not sufficient to compensate the opposite effect due to the gates, and the driven cells are in the incorrect polarization state. It would be possible to increase this value, by varying some features of the layout, however this is not a significant issue, at least compared with the other, much stricter tolerances needed for QCA operation.

Convergence of the previously described iterative procedure is usually achieved with a single iteration, due to the strong localization of the electrons in each dot.

## 4. CONCLUSIONS

We have simulated a complete chain of three QCA cells implemented in GaAs/AlGaAs technology, including the procedure for enforcing the desired polarization state in the driver cell, an issue that had not been previously analyzed in detail. From our calculations we conclude that it is possible, and not too difficult from a practical point of view, to obtain proper operation for a chain of QCA cells, by applying a small enough voltage unbalance to the electrodes defining the driver cell, sufficient for fully polarizing it without a significant perturbation of the driven cells, which will respond only to the electrostatic action of the driver cell electrons. This is a result of the bistable nature of QCA cells and, ultimately, of the Coulomb blockade effect, which is a direct consequence of the discreteness of charge. On the other hand, the need for dummy cells or of additional adjustment electrodes for symmetrization purposes, reveals the existence of a further technological problem for large scale QCA circuit implementation.

### *Acknowledgments*

This work was supported by the European Commission through the QUADRANT project (n. 23362), within the MEL-ARI and IST-FET initiatives.

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