Clocking of molecular quantum-dot cellular automata

Kevin Hennessy and Craig S. Lent[a)]
Department of Electrical Engineering, University of Notre Dame, Notre Dame, Indiana 46556

(Received 9 January 2001; accepted 25 June 2001)

Quantum-dot cellular automata (QCA) may provide a novel way to bypass the transistor paradigm to form ultrasmall computing elements. In the QCA paradigm information is represented in the charge configuration of a QCA cell, which maps naturally to a binary model. Molecular QCA implementations are being explored where the quantum dots in the cell take the form of redox centers in a molecule. Clocking has proved important in QCA cells synthesized so far. Here we examine a method to clock molecular QCA cells which are assembled at an interface. The clocking signals in this scheme originate from wires buried below the QCA surface. We present a simplified model of this clocking method and examine its behavior as a molecular shift register. [DOI: 10.1116/1.1394729]

I. INTRODUCTION

The incredible success of the microelectronics industry has been fueled by a progression of complementary metal-oxide-semiconductor technology based on modifying and scaling one standard paradigm. This method has resulted in orders of magnitude changes in feature size and packing density over time. This trend may reach an end, not due to the limitation of human ingenuity, but rather to a change in the physical laws which govern the device behavior at very small scales. If advancement in chip performance presumes further miniaturization, we must depart from the notion of scaling current architectures and learn to develop new paradigms—nanoscale systems that exploit the laws of quantum mechanics rather than seek to obviate them. It is thus natural to explore the ultimate limits of computing elements composed of individual molecules representing information with a few electrons.

Quantum-dot cellular automata (QCA)[1] parallels classical computing yet accomplishes its functionality in ways which are natural and efficient on a nanometer scale. Binary information is encoded in the charge configuration in a cell composed of a small number of quantum ''dots.'' A dot for these purposes is simply a region in which charge is localized. Each cell has two extra mobile electrons and in isolation has two degenerate ground states. The electrostatic effect of neighboring cells lifts the degeneracy and results in a ''1'' or ''0'' state of the cell. This intercellular interaction involves no current flow between cells.

The ability to have clocked control of regions of cells has proven immensely valuable architecturally.[2] Clocking is accomplished by electrostatically switching the cell from a **null state**, in which cell holds no binary information, through a **switching state**, in which the cell state is determined by its neighbors, to a **locked state**, in which the state is independent of its neighbors. It has been shown that logic, memory, indeed general purpose computing, is possible in this scheme.

Recent experiments have demonstrated QCA cells composed of metallic dots operating at cryogenic temperatures.[3] A majority logic gate, a QCA binary wire, clocked QCA operation, and a single-bit memory have all been experimentally demonstrated. Each cell has only two mobile electrons. Room temperature operation of large arrays of metallic cells may prove beyond the ability of fabrication techniques to achieve junctions with sufficiently small capacitance. A molecular implementation, by contrast, holds the promise of room temperature operation because of the much smaller size scales and corresponding high characteristic energies.

II. CLOCKED MOLECULAR QCA CELLS

Molecular implementations are currently being explored.[4] In a molecular QCA cell the dots are redox centers in a molecule which can be occupied by, for example, one or two electrons (or holes). Some implementations have four redox centers in the molecule, resulting in one molecule per cell. Others use a molecule to construct a half cell with a single mobile charge. For simplicity we will focus on this mode for which there are two molecules in each full QCA cell.

The geometry of the cell allows three distinct states of charge configuration depending on the strength of an electric field applied to the cell. Consider a single half cell as shown in Fig. 1 where the dots are redox centers of a molecule and connections between dots are bridging ligands in the molecule. With a strong positive electric field applied to the cell, the electrons will be drawn into the lower quantum dot, effecting a **null** state that does not participate in computation or hold information. As the field becomes somewhat negative, the electrons will exist in a **switching** state, occupying the upper dots but still able to tunnel through the lower dot and switch their configuration. The effective tunneling matrix element between the two information-bearing states is nonzero. As the field becomes strongly negative, the electrons will be forced up, into the **locked** state and hold a bit of

[a)]Author to whom correspondence should be addressed; electronic mail: lent@nd.edu

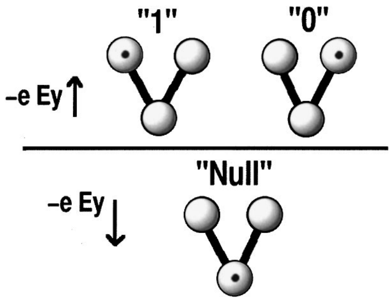

FIG. 1. Cross section of a QCA half cell showing two different states it can exist in. The state is determined by a $\hat{y}$ directed electric field that either pushes the electrons into a locked state, sucks them down into the null state, or switches them in between. The locked state has two degenerate polarities shown here to represent a binary 1 or 0.

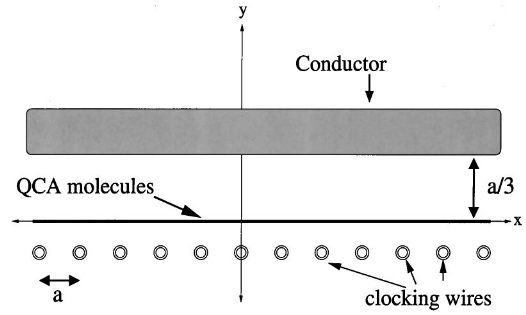

FIG. 3. Schematic of the model we use to represent a large-scale, clocked, molecular QCA array. The QCA surface, containing a line of QCA cells, is found on the x axis. Wires buried under this surface run perpendicular to the page and induce an electric field at the QCA surface when a voltage is applied to them. The electric field in the $\hat{y}$ direction influences the cell's state: null, locked, or switching; and not its polarization: 1 or 0, which will be determined by the cell's neighbor.

information depending on which one of the dots they occupy. At this point the effective tunneling element between the 1 and "0" state is negligible.

Which of the two upper dots are occupied is not determined by the $\hat{y}$ component of the field; only an $\hat{x}$ directed electric field can split the degeneracy. This field is provided by the cell's neighbors and determines whether a logical 1 or 0 is represented in the cell. As a cell is changing from the switching state to the locked state, the electron will occupy the dot that aligns the cell's polarity with its neighbor cell's polarity. Two cells are depicted in Fig. 2 showing how neighboring cells will tend to assume the same polarity.

Our goal is to create an electric field that will induce data flow down a line of QCA cells. We choose to explore how this might be accomplished by using conducting wires below the plane of QCA molecules to generate a suitable electric field at the QCA surface. A schematic of the physical system is depicted in Fig. 3. A single surface of QCA cells is located in the xz plane and a series of buried wires run in the z direction underneath them. Voltages applied to the wires produce an electric field at the QCA surface that affects the cells' activity state (null, locked, or switching). The grounded conductor above the QCA surface serves to draw the electric field lines in the $\hat{y}$ direction, since only this component of the field affects a cell's activity state.

By applying the correct time-varying voltages on the wires, we can clock the cells' activity to produce a flow of information.[5] The voltage signals on the wires are periodic and adjacent wires have a $\pi/2$ phase shift between them, so that every fourth wire will have the same applied signal. The clocking electric field at the QCA surface is referred to as the **clocking field** and the signal on the buried wires that will provide such a field is the **four-phase signal**, which is shown in Fig. 4. This figure shows the voltage signals on four adjacent wires. The shape of the four-phase signal is not a typical square-wave clocking signal, but rather linearly increases and decreases to slowly change a cell's state. If a cell is switched slowly enough, so that the switching time is long compared to the tunneling time between dots, the cell will stay close to its ground state over all time, dissipating little energy. The four-phase signal on the buried wires should induce a roughly sinusoidal clocking field that propagates

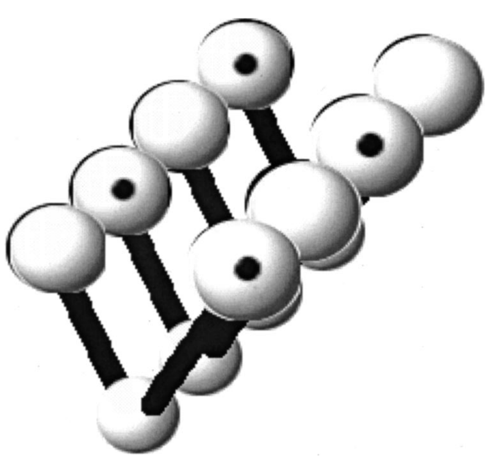

FIG. 2. Schematic of two molecular QCA cells, each with four quantum dots on the top plane used to reflect the polarity of the cell and two dots in the lower plane used to contain the mobile charges when the cell is in a null state. Neighboring cells tend to align their polarities as shown in the figure.

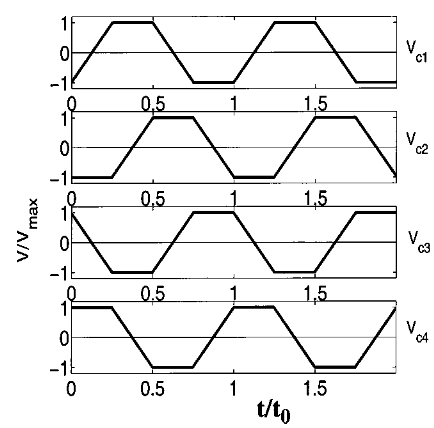

FIG. 4. Four-phase clocking signal applied to four adjacent buried wires. Each wire has a voltage that raises and lowers linearly in order to adiabatically switch the QCA cells above it, that is, switch the cells while keeping them in their ground state. Adjacent wires have a $\pi/2$ phase shift so that every fourth wire has an identical signal. This method will induce a roughly sinusoidal clocking field that propagates along the QCA surface.

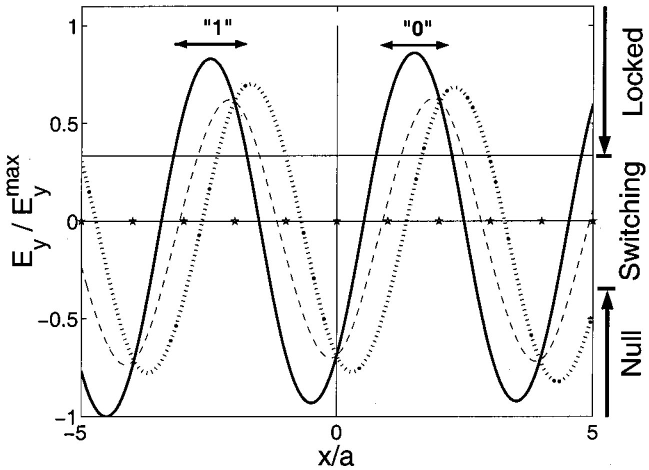

FIG. 5. Value of the clocking field at the QCA surface. Snapshots at different times are depicted by the dotted lines to indicate how the field shifts. Cells on the QCA surface with an applied electric field greater than a critical value will be in a locked state that will be used to store binary information. Over time, the locked state propagates along the *x* axis, transporting binary information.

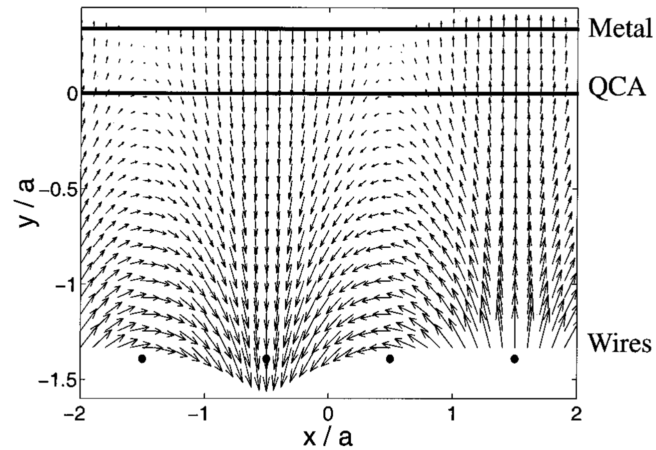

FIG. 6. Electric field distribution between the buried wires and the grounded conductor. The arrows show the direction of the vector field and that the intensity of the field at the QCA surface decreases as it is moved further from the wires.

across the QCA surface. At any region of the surface, the clocking field should cause individual cells to periodically raise and lower their effective tunneling barriers, and at each transition into the locked state, assume the polarization of their neighbor cell. The region of the surface near each clock wire forms a clocking zone influence by the state of that wire. One period of the four-phase clock will cause a string of binary information to shift by one clocking zone, creating a molecular shift register. While we only investigate a linear shift register in this article, this clocking scheme could be used to synchronize general computation across an array of cells.

III. SIMULATIONS

We model the system shown in Fig. 3 with the four-phase signal applied to the buried wires. The goal of the calculation is to verify that buried wires, with the four-phase signal applied to them, will produce a total electric field at the QCA surface that results in data flow along the QCA line. Each wire is modeled as a long line charge with zero radius; this description affords us a simple, analytical solution to the field produced in space by the charge on the wire. The total clocking field at the QCA surface is calculated by summing the fields produced by each wire at every point across the QCA surface for each iteration of time. To account for the grounded conductor, we place image wires into the model and include their electric fields in the summation. Only the $\hat{y}$ component of the electric field is considered since the $\hat{x}$ component does not affect the cell state and the $\hat{z}$ component is zero by symmetry.

The time evolution of the total clocking field produced at the QCA surface is shown in Fig. 5. The strength of the electric field will drive the QCA cells into either the locked, switching, or null states, and these critical values of the electric field are shown in Fig. 5 in relation to $E_y^{\max}$, the maximum amplitude of the clocking field. The critical field value needed to induce either a locked state or a null state, E_{crit}, is dependent upon the exact type of molecules used in the QCA implementation; we pick a value of $E_y^{\max}/3$ for illustration.

In this simulation, $E_y^{\max}$ attains a value of 150 mV/nm but can be adjusted by changing the distance between the buried wires and the QCA surface. The electric field distribution between the wires and the QCA surface is depicted in Fig. 6 and shows that by moving the surface closer to the wires, $E_y^{\max}$ will increase. However, the shape of $E_y(x)$ at the QCA surface will tend to become less sinusoidal as this distance is made smaller.

As the clocking field evolves in time, depicted in the figure by dotted lines in Fig. 5, a considerable width of the roughly sinusoidal wave remains intense enough to induce locking. This region smoothly propagates across the QCA surface resulting in a continuous procession of locked states

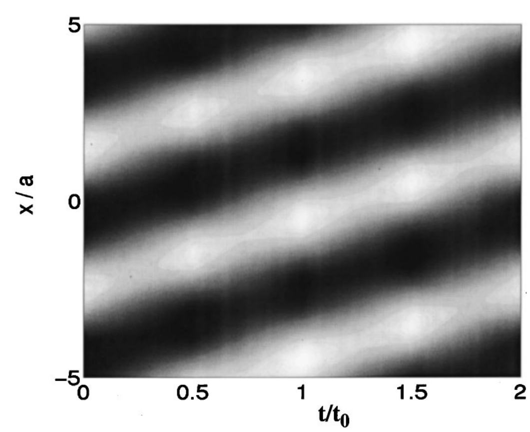

FIG. 7. Electric field at the QCA surface as a function of both time and position. A vertical cross section will show the field at a given time and will be oscillatory as shown in Fig. 5. The bright bands correspond to cells that will be driven into locked states. A continuity of these bands over time ensures that locked states and therefore data will proceed across the surface without interruption.

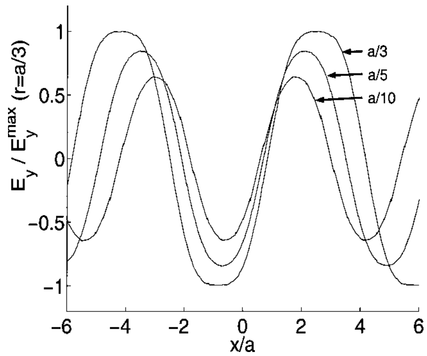

FIG. 8. Electric field at the QCA surface for three different values of wire radius. As the wire radius increases, the amplitude of the field becomes larger since more charge is on each wire at a specific voltage. As the radius decreases, the wave shape becomes more pointed, reflecting the more definite position of each wire underneath the surface.

that will each contain one bit of data. For molecular systems contemplated, the separation between QCA cells on the surface would be between 1 and 2 nm (about $a/10$). As the system evolves in time, any individual QCA cell will change states from locked→switching→null→switching→locked. As the cell is making a transition from switching to locked, it will lock in a new data value corresponding to the value on its neighbor cell, resulting in a transition of data along the entire chain of cells. The smooth propagation of locked states, and therefore data, over time is visualized in Fig. 7, which shows the intensity of the electric field over both position and time; bright areas correspond to a field that is strong enough to induce locking. Any vertical slice through this figure will depict the electric field at one moment of time showing the sinusoidal behavior that is clearly represented in Fig. 5. The bright bands in Fig. 7 correspond to the locked states that proceed across the surface and through time continuously. Any interruptions in the bright bands would correspond to a disruption of data flow.

For this simulation we use a distance between wires, a, of 15 nm; a wire to QCA distance of 4 $a/3$; a QCA to conductor distance of $a/3$; 20 wires; and a voltage amplitude of 5 V. The clock period t_0, referred to in Fig. 7, is limited by the capacitances of the wire network which, though not considered in detail here, could certainly enable speeds of several GHz.

The question arises as to whether treating the wires as zero-radius line charges is too simple an approximation. We check the effect of this by examining the effect of wire radius on the clocking field. Considering the finite radius of the wires requires the numerical solution to the Laplace equation for the geometry studied. The results of the full Laplace simulation closely mirror the previous results, differing only subtly in the final clocking field intensity and shape of the wave. A typical plot of the $\hat{y}$ component of the electric field at the QCA surface for an instant in time is shown in Fig. 8 for three different values of wire radius. Subsequent plots of the electric field show it evolving in time consistent with the clocking field from the simplified wire model, that is, it can sustain the continual motion of locked states across the QCA surface by remaining above $E_{\rm crit}$ in appropriate locations. The finite radius of the buried wires serves mainly to alter the exact shape of the wave form. In both models, however, a smooth propagation of locked states and binary information results.

IV. CONCLUSIONS

In this article we have examined a method for adiabatically clocking molecular QCA cells using buried wires with a four-phase clocking signal. A calculation for an idealized system was performed to verify functionality. Additionally, a second model was simulated that more-closely approximated the physical system by taking into account finite wire radius. Both models showed similar results leading us to conclude that a real system based upon this clocking scheme will continuously propagate locked states across a QCA surface, emulating classical shift register behavior since a binary digit of information can be stored in each cell's locked state.

ACKNOWLEDGMENT

This work was supported by DARPA and the office of Naval Research.

Presented at the 28th PCSI Conference, Lake Buena Vista, FL, 7–11 January 2001.

[1] C. S. Lent, P. D. Tougaw, W. Porod, and G. H. Bernstein, Nanotechnology **4**, 49 (1993).
[2] C. S. Lent and P. D. Tougaw, Proc. IEEE **85**, 541 (1997).
[3] A. O. Orlov, I. Amlani, G. H. Bernstein, C. S. Lent, and G. L. Snider, Science **277**, 928 (1997); I. Amlani, A. Orlov, G. Toth, G. H. Bernstein, C. S. Lent, and G. L. Snider, *ibid.* **284**, 289 (1999); G. L. Snider, A. O. Orlov, I. Amlani, X. Zuo, G. H. Bernstein, C. S. Lent, J. L Merz, and W. Porod, J. Appl. Phys. **85**, 4283 (1999).
[4] C. S. Lent, Science **288**, 1597 (2000); X Lei, E. E. Wolf, and T. P. Fehlner, Eur. J. Inorg. Chem. 1835 (1998); W. Cen, P. Lindenfeld, and T. P. Fehlner, J. Am. Chem. Soc. **114**, 5451 (1992).
[5] G. Toth and C. S. Lent, J. Appl. Phys. **85**, 2977 (1999).