Quantum-dot Cellular Automata by Electric and Magnetic Field Coupling

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Abstract

Even as CMOS technology advances into the nanoscale regime, computing with quantum dots, molecules, or single-domain nanomagnets remains a viable goal in nanotechnology research. Quantum-dot cellular automata (QCA) is a paradigm for low-power, high-speed, highly dense computing that could be realized in a variety of materials systems. This paper reviews the basic paradigm of QCA, discusses various materials systems in which QCA might be constructed, reviews a series of experiments performed in the metal tunnel junction technology, and presents ideas for future QCA implementations in molecules and nanomagnets.

Introduction

Starting in the early 1960's, microelectronics processing technology has traveled two somewhat parallel, unrelated tracks. On the one hand, CMOS technology has marched relentlessly toward ever-smaller geometries. In the ensuing decades, progress in materials growth, as well, led to atomic control in the third dimension, contributing to important technologies in optoelectronics and microwave circuits. Starting around the same time, early research into nanostructures and nanotechnology very quickly produced lateral structures well below a tenth micron (1). Progress on this second, research-oriented track has dealt largely with investigating novel nanofabrication techniques and structures.

Until the early 1990's, this research into nanotechnology still held a firm lead on "future" ultrasmall structures. However, it is clear from the International Technology Roadmap for Semiconductors that industry has already passed the historically "official" boundary of nanotechnology, i.e. 100 nm, with 2003 drawn gate lengths of 65 nm and etched at 45 nm. By 2010, gate lengths of less than 20 nm will be in production. Nevertheless, issues of power dissipation will not go away, and will become possibly the most serious issue facing CMOS IC development.

In the 1980's, much work on quantum devices was performed, with the common prediction that quantum effects would ultimately be the undoing of future nanoscale CMOS transistors, the very same ones discussed above. Toward the goal of exploiting quantum effects, significant effort was put into investigating quantum transport in reduced dimensionality structures. The fact that these phenomena were evident only at very low temperatures did little to deter those who looked toward the demise of CMOS. Part of this work was investigation into the ultimate reduced-dimensional structure, the quantum dot. As alluring as very small devices exhibiting energy quantization and electron wave properties were, the imaginations of many researchers were especially captured by the quantum dot in that it represented the ultimate limit to size scales envisioned for semiconductor devices. The notion of molecules as processing elements was not as yet commonly considered, although some were working toward that goal (2).

Quantum dots were predicted to exhibit interesting cooperative behavior in many-dot systems with overlapping wave functions, due to the resulting miniband structure (3), and also as elements in cellular neural networks (4). However, no scheme for using discrete quantum dots for computing was proposed during this period. In 1987, metal tunnel junction structures exhibiting single electron properties were fabricated by Fulton and Dolan (5). These "dots" were not quantum dots in the energy quantization sense, but rather relied on their ultrasmall capacitance, which was a consequence of their very small size, to reveal measurable voltage changes with charge variations of only a single electron. Such behavior is classical, except for tunneling between dots. In confined semiconductor dots, the energy quantization is superimposed on the Coulombic effects, but are not the primary phenomenon of interest.

In 1993, the notion of quantum-dot cellular automata (QCA), in which quantum dots respond to the charge state of their neighbors, was introduced (6), offering the first computation scheme where quantum dots play the central role in Von Neumann type computing. At that time, it was envisioned that semiconductor quantum dots confined by leaky barriers would lead to QCA architectures (7), but it was found to be cumbersome and prone to charge fluctuations caused by impurities and defects; metal tunnel junctions of the Fulton-Dolan type for charge confinement were found to be easier to fabricate, more reliable, and easier to analyze and model. A set of experiments, reviewed briefly in this paper, resulted from the continued

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refinement of the metal tunnel junction system. However, this serves only as a prototype system, and is subject to several problems of stray charge in the substrate, as well as the inevitable limit to the number of control lines needed to bias the cells. Also, this system functions only at low temperatures. Other, promising systems consisting of molecules and nanomagnets, not subject to the same constraints, will be discussed briefly as well.

What is QCA?

QCA is a transistorless computing paradigm that, rather, exploits interacting electric or magnetic field polarization to effect Boolean logic functions. For charge-based QCA, no current, other than a small displacement current, flows during computation. For magnetic QCA, magnetic dipole interactions effect computing. In this brief introduction we concentrate mostly on charge-QCA. Fig. 1a shows the simplest form of a charge-QCA "wire," in which the basic cell consists of two additional electrons residing on a group of four quantum dots, or other suitable "charge containers," which are assumed to be separated by tunneling paths. In the figure, the left-most cell is influenced by a controlled voltage input. The ground state configuration for a cell is the charge residing on a diagonal, and neighboring cells align themselves to relax to the ground state of the system. The tunneling paths cause a highly nonlinear behavior in the switching characteristics of adjacent cells, so that a polarization "gain" results in switching of adjacent cells. Later variations of QCA in which power gain between cells is achieved as well will be discussed.

Based on this concept, and keeping in mind the lowest energy state of the system (qualitatively determined by merely keeping electrons as far apart as possible), several logic elements can be constructed. Figs. 1b and 1c show a QCA inverter and majority gate, respectively. With one input fixed, e.g. A, the majority gate functions as either an AND gate (A=0) or an OR gate (A=1). Two other necessary elements of a QCA circuit are a fan-out pattern and a wire crossover pattern that allows QCA circuits to be structured in a single plane. Fig. 2 is a QCA single-bit full adder (8). Each of the above logic elements used in the adder are identified by the letters a-e, respectively. Magnetic QCA is qualitatively similar (9, 10), but relies on interacting magnetic dipoles to seek the lowest energy states. In this case, inputs and outputs are addressed by current loops or differences in magnetization energies induced by geometrical effects.

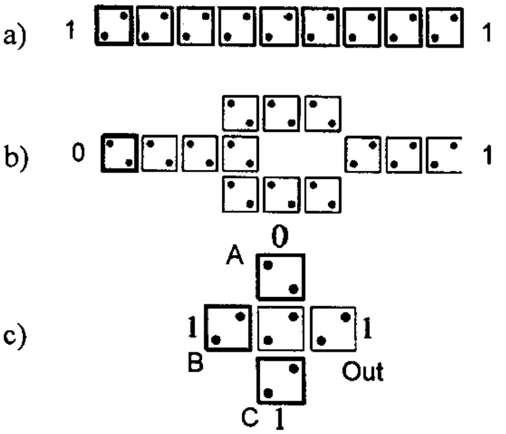

Fig. 1. Three QCA functions. a) wire, b) inverter, and c) majority gate.

An important refinement to the basic QCA concept discussed above is the idea of clocked QCA (8). In such a system, switching of the cells is accomplished at the control of an additional clock signal. In the most general sense, the clock controls the barriers, so that when they are relaxed the electrons are not localized to any particular dots within the cell (but are still confined to the cell). This is called the "restore" phase. The cell may then be biased by input voltages, and as the barriers are raised ("switch" phase), the electrons are preferentially shifted to one end-dot. When the clock is fully raised ("hold" phase), the QCA cell is fully charged and the electrons are latched into their positions even if the input bias is removed.

A variety of material systems are candidates for QCA. These include quantum dots formed in either heterostruc

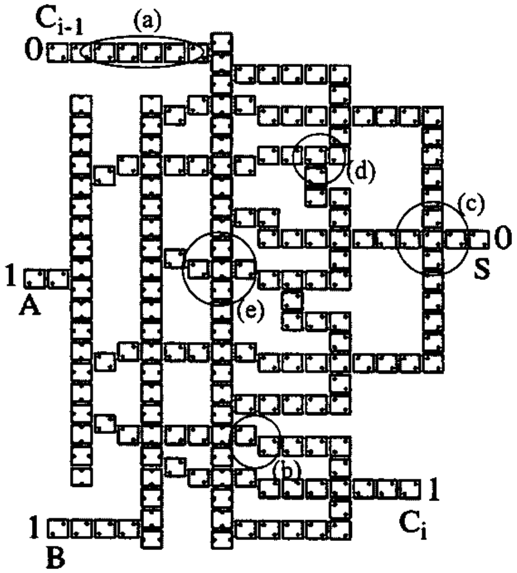

Fig. 2. QCA single bit full adder. The following sections are labeled: a) wire, b) inverter, c) majority gate, d) fan-out, and e) crossover.

ture or Si/SiO$_2$ two-dimensional electron gases (2DEGs). Confinement barriers are created by potentials applied to surface gates, which squeeze the electrons into quantum dot formations. A functioning QCA cell in a GaAs/AlGaAs heterostructure has recently been demonstrated (11) at a temperature of 100 mK. In addition to other issues mentioned above, this configuration is useful only as a prototype system due to the unwieldy number of gates required.

The simpler metal tunnel junction system has been used by the Notre Dame group to demonstrate several basic QCA cell and logic functions. In this system, Al islands are created by an angled evaporation process in which, after electron beam lithography of a double layer resist on SiO$_2$, Al is evaporated, then oxidized *in situ*, and then evaporated again at an angle so that the resulting Al islands are electrically floating between two thin oxide tunneling barriers. Due to the very small capacitance of the island (on the order of 10^{-16} F), a change in the population of even one electron results in a measurable difference in potential. The tunneling of electrons on and off the island can be controlled by an external gate. Such a 3-terminal device is referred to as a single electron transistor (SET). With an external source-drain (SD) bias, ramping the gate voltage causes oscillations in the SD current. At every oscillation, the electron population on the island has changed by precisely one electron. This is a self-limiting process in that after one electron has been added to the island, it is energetically unfavorable for another electron to populate it until the gate bias is changed to allow another electron on. We use SET-like structures as both elements of QCA circuits and as sensitive electrometers to probe the charge state of dots within the QCA system.

The two remaining candidate materials systems for QCA are magnetic materials and molecules that alone behave as entire QCA cells. We will review experiments in metal tunnel junction systems and then discuss progress in magnetic and molecular QCA systems.

Experiments in Metal Tunnel Junction QCA

Metal tunnel junction QCA cells have so far consisted of a series combination of two dots (here, "dots" refers to the metal islands separated by tunnel junctions, on which reside the electrons involved in polarization), capacitively coupled to another pair of dots and up to four SETs serving as electrometers that probe the charge state of the dots. The charge state of the electrometer SETs does not affect the charges on the dots because the SETs are biased to a point of maximum sensitivity, and feedback is used to keep their charge constant. All metal QCA experiments discussed here were performed at approximately 70 mK and with a magnetic field of 1 T in order to avoid thermal and superconductivity effects, respectively.

The series combination of two dots can either be coupled to reservoirs through the bias power supply and ground, or left floating. In the first case, current flows during the switching event of adding or removing an electron, which in itself can be used to determine the number of electrons added to a dot. In the latter case, two dots connected by tunnel junctions may only exchange electrons, the total number being constant.

Fig. 3 is an electron micrograph of a floating metal tunnel junction QCA cell. The four circles to the left indicate the positions of the floating QCA islands, which are extended to coupling capacitors, and the two to the right indicate the electrometers used to probe the charge state of the right two islands of the cell. Two additional electrometers are to the left. The two dots on the left (arbitrarily called "input") are capacitively coupled to the two dots on the right ("output"). The bar represents 1 micron.

In the grounded version, a map of conductance as a function of gate and drain voltage is used in selecting operating points and biasing cells near switching points. Observation of conductance changes provides information regarding the charge state of the dots, and confirms the electron switching observed by the electrometers. As confidence in the electrometer measurements was gained, we moved entirely to the floating dot configuration and relied only on the electrometers to determine the internal charge states of the dots.

Experiments of clocked QCA, in which "barriers" between dots were modulated, were performed as well. Clearly it is not feasible to directly modulate a thin (about 1 nm) oxide barrier layer to control tunneling between dots. Instead, a third version of the metal QCA cell employs an extra dot between the two end-dots. This additional charge-storage site acts as a variable barrier to tunneling between the end-

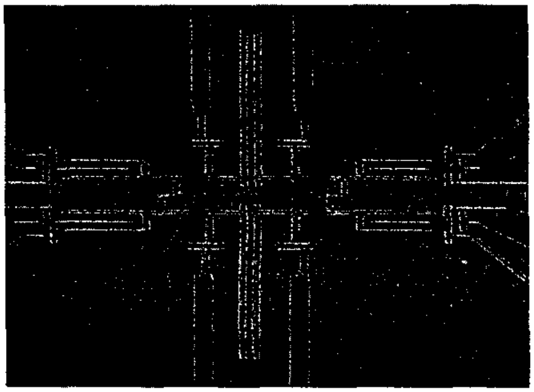

Fig. 3. Electron micrograph of a floating metal tunnel junction QCA cell. The four circles on the left indicate the floating islands connected to coupling capacitors, and the two on the right are electrometers. The bar is 1 micron.

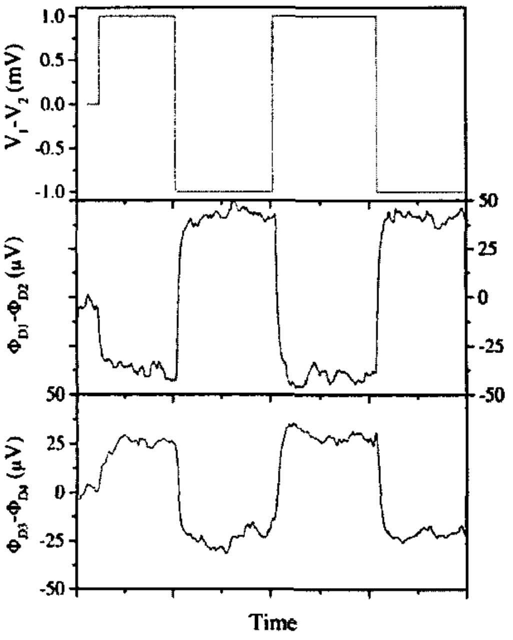

Fig. 4. Switching behavior of a grounded QCA cell.

dots, and the gate control of this middle dot serves as the clock. *In our experiments, we considered two dots in series to be a "two-dot cell" and the three dots as a "three-dot cell."* Putting two, two-dot cells together demonstrated QCA operation, in both grounded and floating systems. Operation of only floating three-dot cells was investigated.

Fig. 4 shows the resulting switching behavior of a grounded QCA cell. As the input voltage V1-V2 is made positive, an electron is attracted to an input dot, D1, making its potential negative, as measured by an adjacent SET electrometer. In response to this switch, an electron is driven off the opposite output dot, D3, making its potential more positive. This is precisely QCA operation.

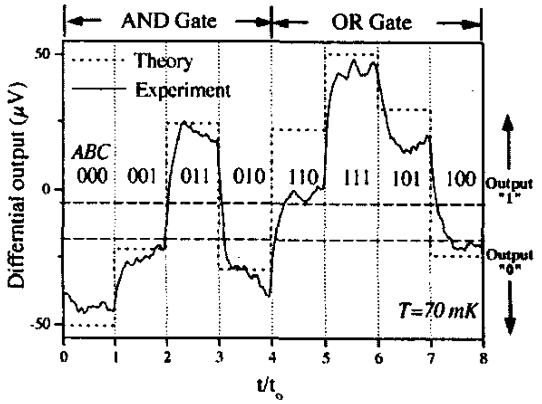

Fig. 5. Behavior of a 4-dot cell configured as the central cell of a majority gate.

Fig. 5 shows the results of a 4-dot cell configured as the central cell of a majority gate (see Fig. 1c). This was accomplished by applying voltages to all four gates of a cell to mimic the biases known by previous measurement to be caused by the various charge configurations of three inputs. *Electrometers were used to observe the charge state* at the output. Note that for half of the eight input combinations, each of the AND and OR functions is demonstrated.

The most complicated system allowed by the limited number of electrical contacts to our cryostat is that of a six-dot, i.e. clocked, cell configured as a QCA shift register. This experiment demonstrates several features simultaneously, namely the use of the clock to control switching in a 3-dot cell, switching in floating cells, charge coupling between cells, latching of electrons in end-dots, two-phase clocking for shift register functionality, and storage of electrons for finite times in the end-dots. This last feature is effected by the use of extra tunnel junctions between the center and end-dots that minimize the probability of the electrons

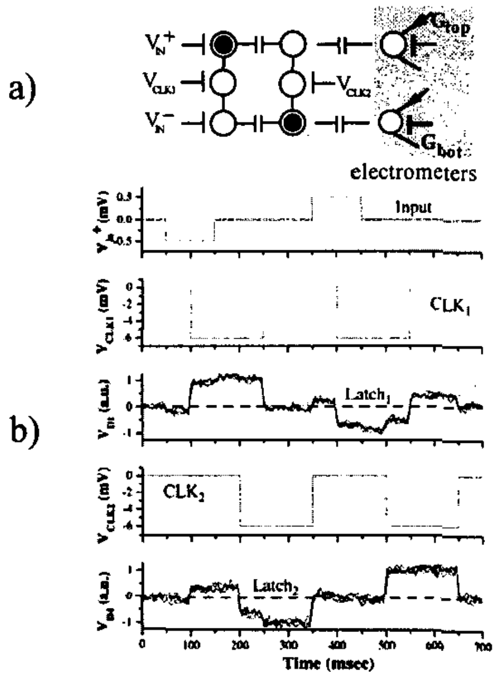

Fig. 6. Test of QCA latch and shift register. a) Schematic of two three-dot cells configured as two latches, with tunnel junctions between dots and capacitive coupling between the two latches. Output is derived from the two electrometers on right. b) Data of input latched first to the left latch and then on the clock signal passed to the right latch.

"leaking out" by the mechanism of co-tunneling (12). Fig. 6a is a diagram of the test structure (including 2 of the 4 electrometers), and Fig. 6b shows the two-phase shift register operation. Except for minimal cross-talk, the behavior of the input and output cells is controlled by the inputs and the clocks, and although the input voltage is removed, the input latch retains its correct charge configuration, which is successfully passed to the second latch.

A detailed examination of power gain in QCA is not presented here. However, it has been demonstrated (13, 14) that it is possible to refresh the logic state of a cell through power from the clock. This solves possible problems of metastability in the unclocked QCA architecture, and suggests schemes in which regions of large QCA arrays can be synchronized to minimize the probability of errors.

Molecular QCA

The ultimate size limit of computing must necessarily be a single molecule. At these size scales, QCA operation at room temperature would be possible with unheard of circuit density, speed, and low power dissipation. Such a notion is within the realm of the possible, as many variations of molecules have been designed that incorporate redox active corners connected by tunnel junctions, as well as chemical moities to serve as surface attachment sites. In these cases, we envision single molecules functioning as whole QCA cells. There are numerous examples of the analogous two-dot cell, for example silicon phthalocyanine dimers (15) as shown in Fig. 7. The HS-group (thiol) is an example of feet that attach the molecules preferentially to a surface, in this case gold. We have demonstrated that a liftoff process of molecules, similar to that commonly used for metals, is possible (16). A requirement for such a process is that the molecules stick to the surface and not to the resist. Also, the molecules must not be soluble in a suitable resist remover. Fig. 8 shows nominally 20 nm lines formed by EBL of polymethylmethacrylate (PMMA) on SiO_2, development, submersion in a solution containing

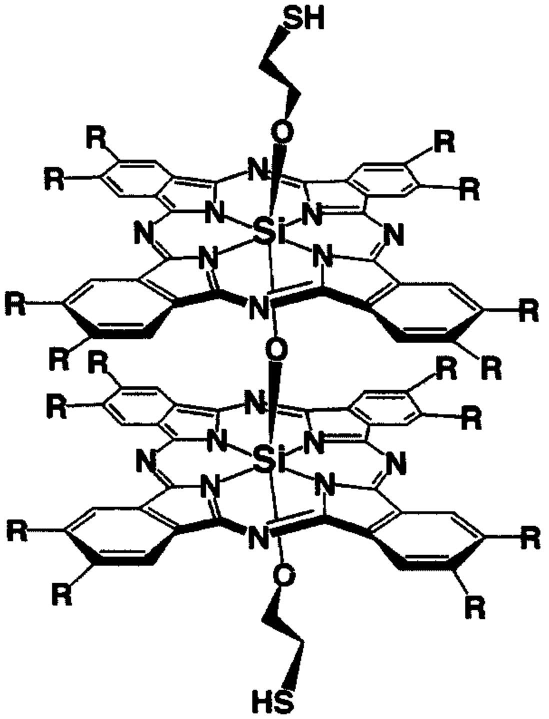

Fig. 7. Model of silicon phthalocyanine dimer under consideration as two-dot QCA cell. The HS, thiol, group allows attachment to gold surfaces.

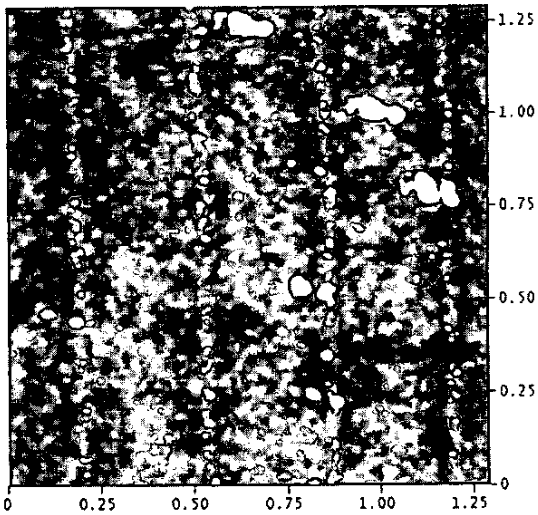

Fig. 8. Atomic force microscope image of lines of CT5 molecules formed by liftoff. The apparent linewidth is about 20 nm. The radius of the AFM tip is estimated to be 10 nm, so the actual linewidth is somewhat smaller.

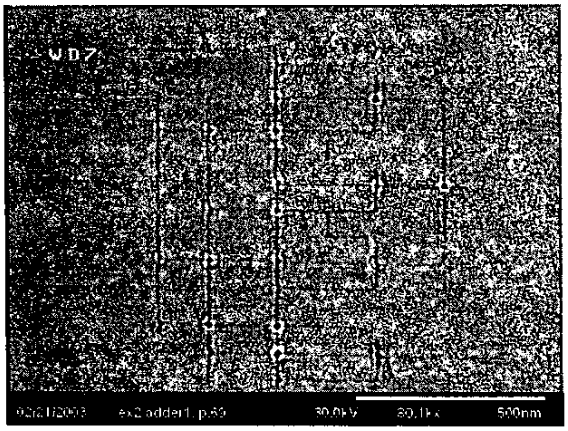

Fig. 9. Demonstration of QCA single bit full adder circuit rendered in approximately 5 nm PMMA lines. Lithography-assisted self assembly of molecules may at some point create full QCA circuits in this manner.

specialized Creutz-Taube molecules (called "CT5"), and removal of the PMMA in methylene chloride for improved surface cleanliness (17). A practical molecular QCA system would consist of lithography at the few nm scale, molecules that attach in the channels, and self assembly in lines to form circuits with sufficiently few errors. As shown in Fig. 9, we have demonstrated EBL of 4-5 nm lines, which as a demonstration is patterned as the adder circuit of Fig. 2. Such lithographic patterning should allow single or double lines of QCA molecules to be formed. Input and output from such arrays could conceivably be performed by advanced nanotube-based devices at size scales commensurate with molecules (18).

Magnetic QCA

The materials and systems architectures discussed above have charge coupling in common. Field coupled nanomagnet arrays, however, offer the possibility of QCA systems exhibiting robust room temperature operation (9, 10). Fig. 10a shows a QCA wire of EBL-fabricated, 25 nm thick permalloy nanomagnets. Fig. 10b shows that even at room temperature there is a propensity for the nanomagnet domains to naturally anti-align (alternating N-S poles). This robustness is promising for nanomagnet QCA.

It is easy to imagine nanomagnet QCA systems based on wire loops for control, and giant magnetoresistance (GMR) devices for sensing. In fact, this area is under investigation at Notre Dame. Since the switching energy is higher ("harder" magnetization) in the shorter direction of a rectangular nanomagnet pillar, the polarization of the first, narrow, pillar in a line could be used to control the resulting polarization of a line of thicker magnets, whose magnetization along the line would be "softer." An external field could align the polarizations along the line, and after the first, harder, magnetization is set by an input current carrying wire, upon removing the external field the polarization of the rest of the line would follow based on the magnetization of the first pillar.

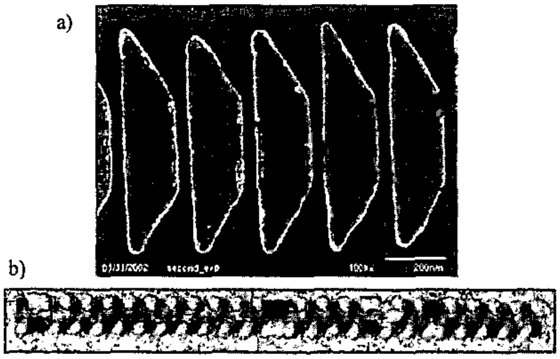

Fig. 10. Field coupling in nanomagnets for QCA. a) SEM micrograph of permalloy nanomagnets and b) magnetic force microscope image showing spontaneous antialigning of magnetic dipoles. This behavior suggests that QCA operation at room temperature is feasible.

QCA Circuits

Some of important issues for QCA include power dissipation, speed, defect tolerance, operating temperature, density, and manufacturability (all of which must ultimately be addressed, so no order of importance is suggested).

Power dissipation: Clocked QCA operates very close to the theoretical limits of minimum power dissipation. For very fast clock speeds, as an electron traverses between the end-dots, it finds itself at relatively high energy, and must thermalize to the ground state. For "adiabatic" switching, i.e. lower clock speeds, the electron stays closer to the ground state and therefore dissipates less energy.

Speed: The absolute limit of switching speed is determined by tunneling times, but the more practical limit to speed is power dissipation. Even with adiabatic switching, clock speeds for molecules could be as high as the THz range. Magnetic QCA is limited by the speed of domain switching, but can also be adiabatically clocked. Operating speeds are expected to be around 100 MHz.

Defect tolerance: The intrinsic bistability of the cell-cell interactions provides considerable tolerance against placement errors. Nevertheless, it is straightforward to implement a triple modular redundancy along the wires.

Density: This is a difficult issue to address since there is not a perfect correspondence between a QCA cell and a logic gate. However, we can make a rough approximation by comparing a majority gate consisting of four cells to, say, an inverter. For molecular QCA, it would be possible to achieve 10^{13} cells cm^{-2}. This far exceeds any current projections for CMOS. Magnetic QCA of 20 nm dimensions would achieve perhaps 10^{11} cells cm^{-2}.

Operating temperature: Molecular QCA has a kink energy, i.e. the energy associated with an error, on the order of an electron volt (40 kT at room temperature), so thermal errors would play a negligible role. For magnetic QCA, the switching energy can be 100's of kT. For nanomagnets smaller than about 10 nm, thermal energy disordering at room temperature begins to dominate.

Fig. 11 shows the data flow of a 1-bit portion of an ALU (19). One of the distinct features of QCA that is evident is the "processing in wire" (PIW) feature that makes computing by QCA very efficient. The basis of PIW is that signals must naturally traverse certain distances along the circuit. In QCA, there is no additional cost to performing logic along the path as the signal is routed.

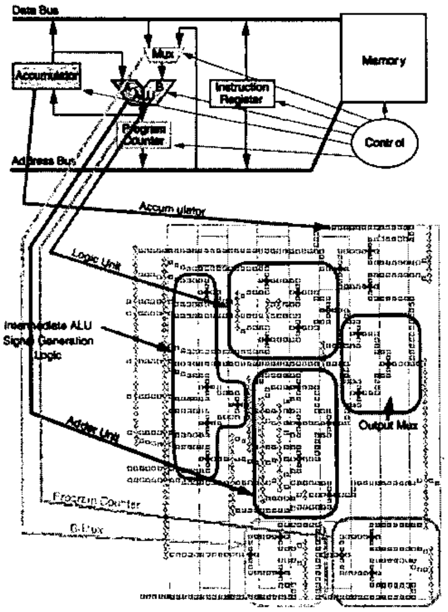

Fig. 11. Data flow of a 1-bit portion of an ALU rendered in QCA.

Summary and Conclusion

We have reviewed the paradigm of QCA and discussed a few experiments in metal tunnel junction and magnetic QCA. Some limitations to the adoption of the technology were discussed. It is likely that the ultimate utility of QCA, in any form, will be in combination with currently existing, advanced technologies, such as CMOS, for the case of molecular QCA, or some totally magnetic technology incorporating logic by QCA and memory by magnetic random access memory (MRAM), for example. As with any research program in an unexplored field, the future utility will likely not be in the precise form studied, but rather from further refinement of the concepts and an evolutionary transformation of them.

Acknowledgments

This paper draws on the work of many of my current collaborators. C. Lent and W. Porod originated the theoretical and architecture underpinnings of the QCA concepts discussed here. G. Snider and A. Orlov led the metal QCA work along with I. Amlani, now at Motorola Labs. P. Kogge led the group working on QCA circuit architectures, and M. Lieberman and T. Fehlner led the molecular electronics effort. The principal graduate student contributors to this research include G. Csaba, Q. Hang, W. Hu, A. Imre, R. Kummamuru, M. Niemier, R. Rajagopal, and J. Timler. This work was supported by Intel, the W. M. Keck Foundation, and DARPA/ONR.

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