A Method to Analyze the Fault Tolerance of Molecular Quantum-Dot Cellular Automata Systems

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Abstract
The Quantum-Dot Cellular Automata computing paradigm (QCA) is based on the electrostatic interaction between QCA cells. Therefore, the correct functionality of the QCA systems strongly depends on the geometrical positions of the cells. Given that during the manufacturing process, the positioning cannot be done with 100% accuracy the question rises by how much the system may deviate from its original geometry before it fails? In this paper we propose a methodology for simulating the effect of positioning faults on the molecular QCA behaviour, which is based on both Molecular Mechanics and Quantum Mechanics approaches.

1. INTRODUCTION

Quantum-dot Cellular Automata (QCA) [1] is a promising concept for building single molecule electronics. It replaces traditional CMOS current switches with QCA cells, where the charge configuration inside the cell holds the binary value. The basic four-dot QCA cell (Figure 1) can be viewed as a square charge container embedding four Quantum Dots (QDs) at the corners. QDs represent islands inside the cell where charge can localize. Two excess electrons are introduced in the cell and due to the Coulomb repulsion between them they always localize on antipodal QDs. Electrons are allowed to tunnel between QDs, but not out of the cell. The ground state of the cell is bi-stable, meaning that two different charge distributions are possible, which we denote as cell polarization P=+1 and P=-1, as depicted in Figure 1. Filled circles represent dots occupied by an electron, whereas empty circles represent unoccupied dots. Although polarization states of an isolated cell are equal in energy, they are ”observables” and can be used to encode a bit of information as follows: positive polarization represents binary ”1” and negative polarization represents binary ”0”. When two or more cells are put close to each other, the two polarization states are not energetically equal thus a QCA system relaxes in the state with the lowest energy, meaning that either the ground state P=+1 or P=-1 is preferred. This is due to the electrostatic coupling between the cells composing the system.

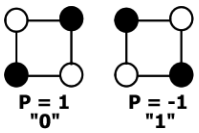

Fig. 1. Four Dot QCA Cell

Basic Boolean gates, e.g., AND, NOT, OR, can be constructed [2] by placing QCA cells together in particular geometrical configurations and their correct functionality strongly depends on the geometrical positions of the cells. Positioning the cells is thus the key issue in constructing reliable QCA based circuits and systems and it is reasonable to expect that this cannot be done with 100% accuracy. Given that these positional errors are unavoidable it is of interest to study the reliability of QCA computational structures to geometrical errors induced by the fabrication process. The reliability in this context means: *How far may a QCA system deviate from its perfect geometry before it fails?* In other words: *What is the fault tolerance of a QCA system on errors in the topology?* A methodology for finding the answer to this question constitutes the subject of this paper. As molecular QCA appears to be the most promising approach towards the fabrication of QCA circuits and systems we tailor our methodology for it.

The remainder of this paper is organized as follows: Section 2 presents basic QCA logic devices and a possible molecular implementation is introduced in Section 3. Fault models for QCA deposition phase are discussed in Section 4. The methodology we propose for simulating error tolerance in molecule placement is presented in Section 5 and simulation results on a majority gate are presented in Section 6.

2. QCA DEVICES

To perform binary computations we need to construct QCA logic gates and a way to distribute

information between them. A QCA *binary wire* is simply formed by juxtaposing cells in a linear array as depicted in Figure 2(a). In this figure input cells have thick borders and output cells have dashed borders. When the polarization of the input cell changes, Coulomb interaction forces nearby cells to take on the same polarization. In this manner a binary value is propagated from the input to the output of a binary wire.

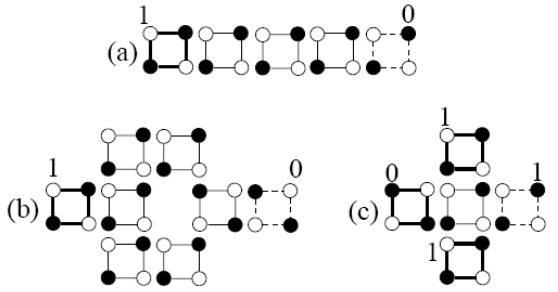

Fig. 2. a) Binary Wire b) NOT Gate c) Majority Gate

Figure 2(b) depicts a schematic of a QCA inverter. Corner interaction between cells positioned diagonally from each other has anti aligning as effect. Therefore the ground state of the output cell is the opposite of the ground state of the input. The three input *majority gate* (Figure 2(c)) is a fundamental logic gate in QCA. It is also called *the voter*, meaning that the central cell is in its lowest energy state when it takes on the polarization of the majority of the inputs. By fixing one of the inputs at logic ”1” the majority gate acts as an OR gate, otherwise if one of the inputs is fixed at ”0” it functions as an AND gate.

With AND, OR, and NOT logic gates we have a full Boolean logic gate set, and with the binary wire information can be distributed. These are all the building blocks needed to construct more complex logic and even simple microprocessors [3] have been designed within the QCA paradigm.

3. MOLECULAR IMPLEMENTATION

The ultimate limits of electronic device miniaturization and integration can be reached by molecular implementation of QCA cells (MQCA). Predicted MQCA device densities are of order 10^{14} per cm^2 for $1nm^2$ devices. In theory, if the cells are 20 to 30Å per side, room temperature (RT) operation of MQCA devices is possible. Moreover, MQCA cells can be made identical through chemical synthesis, meaning that there is no device variation that might have a negative effect on performance. Redox centers inside a molecule serve as QDs. A redox center is an atom or a group of atoms inside a molecule that can gain an electron or loose one without breaking the bonds. Redox centers are connected via a bridging ligand, which serves as a path through which charge is exchanged.

The most interesting molecule proposed so far to serve as QCA cell [4] is depicted in Figure 3.

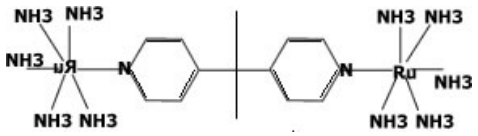

Fig. 3. Creutz-Taube Ion

The molecule in Figure 3 is the so called ”Creutz-Taube” ion, with a total net charge of +5q, where q represents the charge of an electron. The two Ruthenium atoms at far sides of the molecule operate as QDs so each molecule has two quantum dots. It was shown in [4] that when an input is applied charge distribution in the molecule changes accordingly. As a single molecule implements a half MQCA cell, two of them are needed to construct a four-dot QCA cell.

4. FAULT MODELS

Defects in MQCA manufacturing may occur during deposition and are explained with the aid of Figure 4. A schematic of a fault free majority gate is depicted in Figure 4(a) where the centers of all cells are located on either the X or the Y-axis. The possible deposition faults can be categorized as follows:

Cell displacement: a cell is misplaced from its original position such that its center is still on the original axis (Figure 4(b)).

Cell misalignment: is similar to cell displacement, but now the center of the cell is not any longer on the original axis as depicted in Figure 4(c).

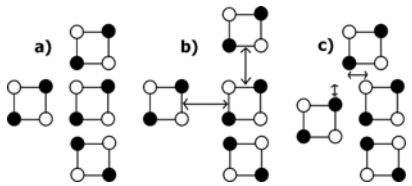

Fig. 4. a)Fault Free b) Displacement c) Misalignment

5. SIMULATION METHODOLOGY

The objective of this work is to model the fault tolerance of MQCA systems to deposition faults.

The molecule that we concentrate on is the Creutz-Taube ion presented in Section 2. The molecule contains two Ruthenium (Ru) atoms, which are 11.5085Å apart and serve as redox centers. By combining two molecules a single square four-dot MQCA cell is formed. To achieve our goal we need to keep track of electrons in the molecules as the binary values represented by the cells depend on which dots the charge is localized. Computing charge densities is the field of *Quantum Mechanical Computational Chemistry* for which different theories exist [5] and tools have been designed that implement them. For our investigation we decided to utilize DFT simulations that give the total charge density of the molecule(s) in the system. However, knowing the charge density is of no direct use. To determine the state of the MQCA cells we need to know the charge of the atoms, especially the charge of the redox centers as they give the polarization of the MQCA cells. Moreover, the concept of charge on an atom inside a molecule is not an observable, as charge cannot be assigned to individual atoms. To deduce the charges we utilize Hirshfeld charge analysis [6].

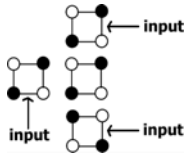

Fig. 5. Ideal Simulation

In an ideal simulation, molecules should be geometrically positioned to form QCA devices. Afterwards, to perform computations, an input to the system is applied as depicted in Figure 5 for a majority gate. This can be an electric field that only acts on the input cells. To evaluate the new state of the system the charge distribution across it has to be computed by means of simulation. By analyzing charge population on the redox centers, the binary value that the cell represents can be extracted. This simulation can be done for various topologies and by using the fault models introduced in Section 4 the tolerance of any particular MQCA system can be analyzed.

For example, assuming the majority gate and displacing the input cells the effect on the charge movement in the output cell can be simulated.

The main problem with this approach is simulation time. Methods, such as DFT, are computationally demanding and for large systems the simulations would take years to complete as the computation time grows exponentially with the number of molecules. Consequently, we have chosen another approach that does not completely rely on DFT simulations as explained next.

When performing simulations of any kind of system, in general there is a trade off between simulation time and the quality of the results. In the case of QCA the results obtained from DFT are superior to those produced by Molecular Mechanics (MM) [5]. On the other hand DFT requires excessive computational time when compared to MM. Our strategy is to combine the best of both worlds such that the required simulation time is low in respective to DFT and the results are superior to that of MM. To achieve this goal we propose to split the simulations in two parts: the first part is done with DFT and the second part with MM.

To be able to evaluate the new state of a MQCA system the most important question to answer is how a molecule reacts to a driver, which may be an input or another polarized molecule. In other words, what amount of charge shift between the redox centers does a driver induce inside a molecule and what is the charge on the atoms in case the molecule is polarized in ”+1”/”-1” state? This question can only be answered by performing DFT simulations as MM ignores electrons. Once the atom charges in the cases of the two polarization states are known the simulations can be continued with MM in two steps. First an MQCA system is constructed where the output represents the correct value and its total energy $E_{faultfree}$ is computed. Following the energy of the system where the output represents the erroneous value E_{fault} is computed. The energies are compared and as long as $E_{faultfree} < E_{fault}$ the conclusion can be drowned that the system functions properly as the laws of physics state that any system settles into a state with the lowest energy. By performing such simulations on systems with disrupted geometry their fault tolerance can be deduced.

6. SIMULATION RESULTS

This section presents simulation results, for deposition faults in the majority gate, obtained by following the methodology introduced in the previous section.

The first step is to compute the charges of Ruthenium atoms, which are expected to act as

redox centers, via DFT simulations performed with the *ADF* simulator [7]. Under the influence of an electrostatic force, charge shift between the redox centers is anticipated. In this simulation an input is emulated by a point charge as indicated in Figure 6. As it can be observed in Figure 6, a driver induces a polarization on the molecule and practically an equal amount of charge is shifted between the redox centers in both cases.

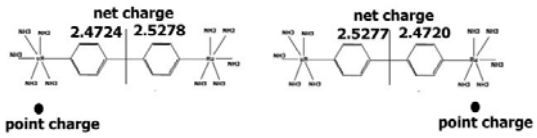

Fig. 6. Net Charges Under a Driver Influence

Following, MM simulations are performed with the *Hyperchem* simulator [8] using the MM+ forcefield.

If we assume that the self-assembly process is able to place the molecules in any direction, several layouts for majority gate are possible. Four of them are depicted in Figure 7. Empty circles represent the molecule dots and the thick lines bridging ligands connecting them. Thus two circles and a thick line between them rare an abstraction of a molecule. A single MQCA cell is formed by two molecules 11.5085Å apart, connected by dotted lines. X, Y and Z are the three inputs of the majority gate.

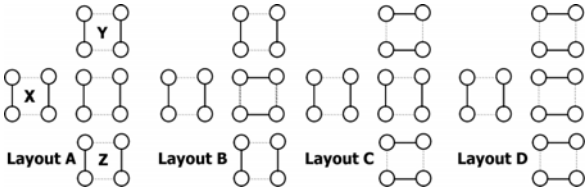

Fig. 7. Possible layouts of the majority gate

In *Layout A* (LA) all cells are placed parallel to the vertical axis in the figure. Central cell in *Layout B* (LB) is rotated by 90° in respect to the central cell in LA. Inputs Y and Z are placed parallel to horizontal axis in *Layout C* (LC). All cells, except X, have vertical orientation in *Layout D* (LD). Cell X is chosen as programmable input that forces the gate into AND/OR logic operation. Two input sets are used throughout the simulations. Displacement of Y and misalignment of X have X ="1", Y ="0" and Z="1" as input. For other cases, X ="0", Y = "1" and Z ="1". The maximum allowed displacement and misalignment for the MQCA cells are reported in Table 1.

	LA	LB	LC	LD
Max. disp. X(Å)	5.7	2.9	4.8	1.3
Max. disp. Y(Å)	1.1	2.9	2.3	4.9
Max. disp. Y and Z(Å)	7.8	3.4	5.8	1.5
Max. disp. CC(Å)	7.8	9.5	9.5	9.8
Max. mis. X(Å)	**0.8**	**1.0**	**0.8**	1.0
Max. mis. Y(Å)	3.0	1.2	1.4	**0.4**
Max. mis. Y and Z(Å)	6.9	6.3	7.5	4.5

Table 1. Maximum Allowed Displacement and Cell Misalignment

7. CONCLUSIONS

In this paper we studied the effect of positioning faults on the molecular QCA behaviour. Our simulations performed on four possible MQCA majority gate layouts indicate that the majority gate is most sensitive to input Y misalignment in the LD layout. Additionally, the tightest constraints to placement errors (given in bold in Table 1, for each layout) suggest that LB is the most robust layout with a maximum allowed input X misalignment of 1.0Å.

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