A Weakly Fault Tolerant Design of Molecular Memory Cell

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***Abstract*—A Verilog-A based model for molecular devices is developed and used to emulate the behavior of molecules like rotaxanne, catanne, nitro containing oligo, etc. A 1-bit molecular memory cell based on nanocell approach is simulated for varying number of nanoparticles and molecular switches. A nanocell consists of nanoparticles interconnected via molecular switches. The presence of multiple paths from input to output increases the probability of getting correct output. A nanocell based memory configuration with Address, Write/Read, Data In and Data Out lines is proposed and verified for functionality. Such a memory can be read, written and erased a number of times. This nanocell based molecular memory is omnipotently trained using genetic algorithm.**

***Index Terms*—nanocell, molecular device modeling, omnipotent training, genetic algorithm, memory design, reliability, fault tolerance.**

I. Introduction

For memory device of dimensions in the nanometer range, performance and reliability is determined by few electron-phenomena. In this context, use of organic and polymer molecular structures may offer some advantages in the long term for future memory applications [1]. Such molecular devices may be economically processed through chemical self assembly and synthesis. Emerging molecular crossbars technology offers advantages like high density, regular, array-like non-volatile memory structure. These devices consume low power, offer low programming voltage and high switching speed. Non-volatility feature permits such memory to be used as programmable elements within a logic device. Researchers have demonstrated the switching behavior of the molecule and have constructed simple logic functions and memory using such programmable molecules [2], [3]. These bistable molecules form active molecular switches, which are used for bit storage in crossbar molecular memory. The bit size is defined by diameter of the molecule and intersecting nanowires. However, the bottom-up approach employed for device fabrication at nanoscale, lacks the precision in the molecular device ordering. The programmable nanocell based approach [4] circumvents this problem. In contrast to molecular crossbar devices, a Nanocell [4]–[7] consists of conducting nanoparticles connected via randomly placed molecules and addressed by relatively small number of leads located at the edges. As demonstrated by Husband *et. al.* [5], a nanocell is omnipotently trained using genetic algorithm to work as combinational logic circuits and bistable latches. In this manuscript, we have omnipotently trained [4] the nanocell to behave as a memory element using genetic algorithm. For designing a nanocell, initially the molecular device model is developed using Verilog-A. The model is based on empirical equations that depict the I-V characteristics of a molecule [8]. The single bit memory cell is simulated in HSPICE. The work is further extended to design of multiple bit memory.

The paper is organized as follows. In Section II, we present background efforts towards implementation and evaluation of nanocell based molecular memory. This includes a brief discussion on basic concept of nanocell based approach and molecular device modeling. We also review the previous attempts done so far. In Section III, we have explained the probabilistic analysis of single input single output nanocell buffer. The nanocell based molecular memory design and simulation results are presented in Section IV. We present conclusion in Section V.

II. Background

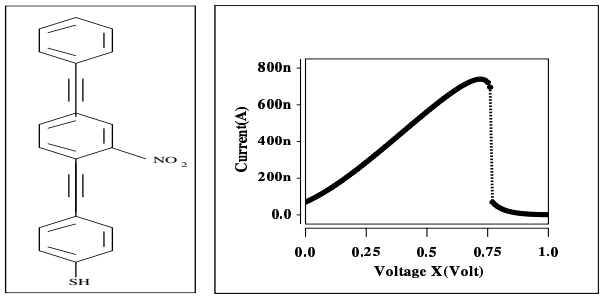
A. Nanocell based approach

The nanocell is comprised of nanoparticles interconnected to each other by molecular switches. These molecules are randomly distributed within the nanocell and exhibit reprogrammable NDR (Negative Differential Resistance) characteristics. At the edge of the nanocell, adequate numbers of lithographically defined access pads are provided to communicate with macroscopic world. The spacing between nanoparticles can be controlled by self-assembly. A monolayer of alkanethiols that coats each nanoparticle, prevents them from coalescing into a multi-particle array. A typical nanocell would contain 250-1000 nanoparticles and 750-10,000 molecular switches approximately. Tour *et. al.* used gold nanoparticles of diameter 60nm and spacing of 3nm. The size of a typical nanocell is approximately $1\mu m^2$. The postfabrication training of a nanocell (omnipotently or mortally [4]) can be formulated as an optimization problem. The optimization process would require as an input the nanocell to be trained, the target logic in

the form of a truth table and the I-V characteristics of the 'ON' and 'OFF' states of the molecular switch. Search space for omnipotent training would include all possible combinations of on and off molecules and all possible assignments of input and output pins. The in-built defect tolerance, small size, postfabrication programmability through mortal training and lack of requirement of precise molecular ordering features makes it a good choice for future nanoscale devices.

B. Molecular Device Modeling

Ziegler *et. al.* proposed an empirical model of molecular switch that masks underlying physics, known as Universal Device Model (UDM) for nanoelectronics circuit simulation [9]. Such molecular switches exhibit non-linear or rectifying current-voltage characteristics. This behavior can be modeled using SPICE or Verilog-A. The UDM model was further revised and more sophisticated models were proposed [8], [10]. We have designed the molecular device model using Verilog-A, similar to UDM device model approach [10]. This device model can be used to capture the I-V characteristics of a molecule behaving as a linear or a non-linear diode or negative differential resistance. The nanocell based memory has been designed using the device model of gold nanoparticles and nitroaniline molecular switches. The Verilog-A model of nitroaniline molecule gives the I-V characteristics as shown in Fig. 1(b) which almost matches to actual molecule curve as reported in Fig. 3 of [4]. The NDR model of the molecule proposed in [7] shows the I-V curve in Fig.6 of [7] which is similar to our curve. The empirical model used here is general and can be used to fit any curve. This flexibility lacks in model proposed by [7].



(a) (b)

Fig. 1. (a)Nitroaniline molecule (b)I-V curve obtained using device model

C. Our Contribution

In this paper, a nanocell based molecular device is omnipotently trained to work as a memory. The probabilistic analysis of nanocell devices is done using MATLAB. An algorithm is designed that calculates the probability of presence of at least one path from input to output. The nanocell based memory cell is simulated for fixed number of nanoparticles (10) and random number of molecular connections among these nanoparticles. The memory is simulated for 300 random configurations. It has been observed that such a memory is more prone to stuck-at-1 fault. The presence of multiple paths from input to output makes such a memory fault tolerant.

III. Probabilistic Analysis of Fault Tolerant Nanocell

A nanocell may have multiple paths connecting input to output ports. At least one of the minimal path must be present between these ports. This is a necessary condition for correct functioning of the nanocell based device. It is sufficient to have multiple paths from inputs to output and some of which may or may not intersect. Multiple paths introduces redundancy and thus we can say that this nanocell based memory is fault tolerant. Even if on some paths, say δ molecules turns to 'off' state due to some transient errors, still the bit storage functionality will be unaffected.

Let us model the nanocell as a planar graph G(V,E), where nanocells are the nodes and molecular switches in 'ON' state are the edges. The graph G(V,E) is assumed to be a directional graph such that all the molecules are oriented in same direction, i.e. from input ports to the output. The primary input node is the root vertex and primary output node is the leaf vertex of the graph G(V,E). Consider a Nanocell with 'n' nanoparticles and 'm' molecular switches. Let us suppose that a nanoparticle is always present and state of a molecular switch i is a random variable such that

$$P\{X_i = 1\} = p_i, \ \ \forall i = 1 \text{ to m}$$

In other words, a molecular switch i is present in 'ON' state with probability p_i. This probability that i^{th} molecule is present in 'ON' state is called reliability of that molecule, denoted as $r(p_i)$. It is assumed that only single edge is present between any two nodes. (Note: In actual nanocell, there can be multiple edges between two nanoparticles and these molecular switches can be oriented in any direction). So, the probability that there is no edge (or connection) in between two nodes (or nanoparticles) is $(1-p)$. Again, the probability that at least one edge is present between two nodes is given by:

$$P\{X_i \geq 1\} = 1 - (1 - p_i), \ \ \forall i = 1 \text{ to m}$$

To begin with, consider a small nanocell with three molecular switches and three nanoparticles as shown in Fig. 2(a). Here, input voltage is applied on A and received on C and this can be done via two minimal paths, namely, AC or ABC. Correct output will be received on C via path ABC if both molecules M_{e1} and M_{e2} are present. Similarly, data will be correctly received on C via path AC if the molecule M_{e3} is in 'ON' state. These are the two redundant paths and at least one of them should be working correctly to obtain correct output. Thus, the probability of receiving correct data on node C is

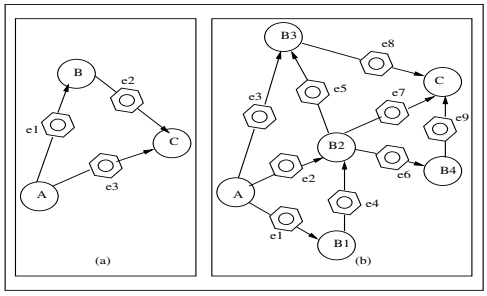


Fig. 2. A small network of nanoparticles and molecular switches(a) example 1 (b) example 2

given by

$$\begin{aligned} P_{path} &= \text{(Probability that at least one molecule between AB and BC) or (Probability that at least one molecule between AC)} \\ &= 1-(1-p_{e1}p_{e2})(1-p_{e3}) \\ &= p_{e3}+p_{e1}pe2-p_{e1}p_{e2}p_{e3} \end{aligned}$$

In this example, the nanocell is working as a buffer. The low and high voltage applied on input node A are $0.5\ V$ and $2.0\ V$, respectively. Table I shows the low and high voltage values received on node C when either none or some of the molecules are missing. Out of eight test cases, correct output is received for five cases only. In other words, $5/8 = 0.625$ or there are 62.5% chances of getting correct output voltage. Theoretically, if $p_{ei} = 0.5\ \forall\ i\ =\ 1, 2, 3$, substituting in above equation, we get $P_{path} = 0.625$. Thus, our theoretical and experimental results are matching. The last three cases in the Table I denotes the minimal cut sets for this nanocell, denoted by, $C_1 = \{e_2, e_3\}$, $C_2 = \{e_1, e_3\}$ and $C_3 = \{e_1, e_2, e_3\}$. As depicted from the Table I, incorrect output voltage is received for these cases.

TABLE I
SIMULATION RESULTS FOR NANOCELL OF FIG. 2A WHEN NONE OR SOME OF THE MOLECULES ARE MISSING

Missing Molecules	V(low)	V(High)	P_{path}
None	0.4935	1.9935	0.625
e1	0.4951	1.9951	0.500
e2	0.4951	1.9951	0.500
e3	0.4902	1.9902	0.250
e1, e2	0.4951	1.9951	0.500
e2, e3	0	0	0.000
e1, e3	-0.4805	-0.4805	0.000
e1, e2, e3	0	0	0.000

Thus, to evaluate the reliability of a trained nanocell, we assume that there are k redundant paths from input to output. Each of these paths may vary in length. The length of any path i can be represented by variable l_i, $\forall i = 1\, to\, k$. That is, each path consists of l_i molecules connected in series and such k paths are working in parallel. For correct functioning of the system, at least one of the i paths must function correctly. Consider an indicator variable x_{ji} which denotes the state of molecular switch j on path i.

$$x_{ji} = \begin{cases} '1' & \text{if molecule is 'ON',} \\ '0' & \text{otherwise.} \end{cases}$$

We define a structure function [11] $\phi(x)_i$ for path i as

$$\phi(x)_i = \prod_{j=1}^{l_i} x_{ji} = \phi_i \qquad \forall i \text{ = 1 to k}$$

Then, structure function of the whole system can be given as:

$$\begin{aligned} \phi(X) &= max(\phi_1, \phi_2, \ldots, \phi_k) \\ &= 1-\prod_{i=1}^{k}(1-\phi_i) \end{aligned}$$

Consider Fig. 2(b) as an example. The node A is input and node C is output. The set of minimal paths from A to C are x_3x_8, $x_2x_5x_8$, $x_2x_6x_9$, $x_2x_6x_9$, x_2x_7, $x_1x_4x_7$, $x_1x_4x_6x_9$, $x_1x_4x_5x_8$. Then at least one of the minimal path from A to C must be present to receive correct output at C. This can be defined as necessary condition for a workable nanocell. It is sufficient to have more than one path from A to C. The structure function for this system is given as:

$$\begin{aligned} \phi(X) &= max(x_3x_8, x_2x_5x_8, x_2x_6x_9, x_2x_7, x_1x_4x_7, \\ &\quad x_1x_4x_6x_9, x_1x_4x_5x_8) \\ &= 1-(1-p_3p_8)(1-p_2p_5p_8)(1-p_2p_6p_9)(1-p_2p_7) \\ &\quad (1-p_1p_4p_7)(1-p_1p_4p_6p_9)(1-p_1p_4p_5p_8) \end{aligned}$$

Hence, the reliability of system [11] at any instant of time is given as:

$$r = p\{\phi(X) = 1\}$$

If all molecules are assumed to be independent, the reliability of individual molecule ($r(p_i)$, $\forall i$ = 1 to m) can be expressed as r, i.e., $r(p_i) = r$.

IV. EXPERIMENTAL SETUP AND SIMULATION RESULTS FOR NANOCELL BASED MOLECULAR MEMORY

As an initial attempt, a 1-bit molecular memory is designed using nanocell based approach. Fig. 3 shows schematic of a nanocell based memory which has an Address Bit, Write/Read, Data In and Data Out ports. When Address Bit is high and the memory is in write mode, the data on the Data In port is stored to the memory. Now, when the memory is switched to read mode, the data stored in the memory can be read out from Data Out port. First, a nanocell is designed in spice using verilog-A model of the nitroaniline molecule, as described in Section II. For molecular connections, the following assumptions are made:

1) Molecules are directional and forward pointing.
2) Between two nanoparticles, only single molecular connection is available.

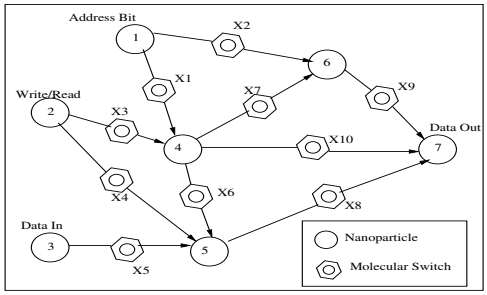


Fig. 3. Nanocell based 1 - bit Molecular Memory Schematic

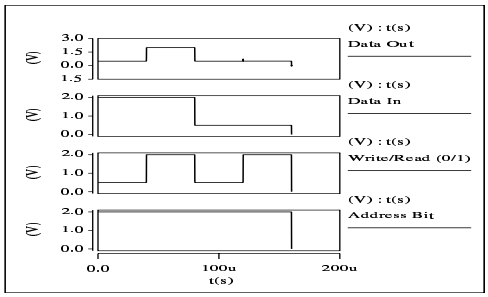


Fig. 4. Simulation results of a 1-bit molecular memory

3) Molecules are randomly distributed within the nanocell.
4) Fixed number of nanoparticles are present inside the nanocell.

A MATLAB code is designed that generates a directed acyclic graph for molecular connections with assumptions stated above. For 10 nanoparticles, normal distribution function has been applied that randomly generates the molecular connection matrix. This matrix has been used in spice code for making initial molecular connections. This spice file is trained omnipotently using genetic algorithm and then simulated for (w1,r1)(w0,r0) operations. The mean value is taken as 1 while variance is changed after every 100 simulation runs. The simulation results for a 1-bit molecular memory with 10 nanoparticles, are shown in Fig. 4. The spice file has been simulated for (w1,r1)(w0,r0) operations.

A total of 300 simulations have been done and results are analyzed. For each of the test cases, a different connection matrix is used. For read 1, the voltage value varies from 1.995 to 1.987. The read 0 values are approximately 0.5 for majority of the cases. The histogram in Fig. 5 shows that there is no test case with stuck at 0 fault, but for few cases, stuck at 1 fault is present. However, might be for some other connections between nanoparticles, the stuck at 0 fault may also occur.

V. Conclusion and Future Work

The molecular device modeling approach using Verilog-A has been presented here. The approach is empirical and flexible to fit any other molecule's transport characteristic. The spice model of the nanocell using the device model of nitroaniline molecule is developed. This nanocell is omnipotently trained

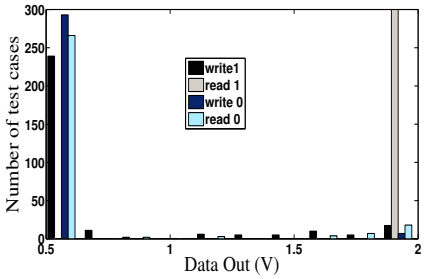


Fig. 5. Data Out of 1-bit memory for 300 test cases

to exhibit the behaviour of a 1-bit memory with read, write and erase capability. The multiple paths from input to output add redundancy to the nanocell device. As a future work, we are developing power and delay model for these memory units. Also, the memory cell is to be extended to store multiple bits of data.

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