DEFECT-TOLERANT MOLECULAR ELECTRONICS

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ABSTRACT

The integrated circuit, manufactured by optical lithography, has driven the computer revolution for three decades. If we are to continue to build complex systems of ever-smaller components, we must find a new technology that will allow massively parallel construction of electronic circuits at the atomic scale. Our Hewlett-Packard and University of California research team is currently developing the molecular electronics building blocks and computer aided design algorithms for a defect-tolerant reconfigurable architecture which allows one to electrically download the designed complexity of a computer into a chemically assembled regular but imperfect nanostructure.

1. INTRODUCTION

Molecular-scale electronics is most likely to be realized with a reconfigurable architecture [1]. Reconfigurable electronic circuits, such as Field Programmable Gate Arrays (FPGAs), are based on configuration bits. A configuration bit is a memory bit controlling a switch. In CMOS technology, configuration bits are constructed from six or seven transistors. With molecular electronics a configuration bit can be a single molecule.

Our proposed technology uses both chemistry and computer science. We use chemistry to thermodynamically assemble highly regular nanometer scale structures. We use computer aided design (CAD) algorithms to download complex electronic designs. We download these designs by opening and closing molecular scale switches. Although the chemically-assembled structures will sometimes be defective, the CAD algorithms are defect tolerant, making the integrated circuits usable [2].

2. Molecular Configuration Bits

A molecular electronics configuration bit is a molecular-scale memory bit that opens or closes a switch. Existing CMOS based reconfigurable logic uses two wires (address lines) to configure the switch, while two different wires (data lines) are used to read it. For the molecular-based switches, only two wires are necessary to achieve both these functions. One voltage is applied to read the device, while a different voltage is applied to configure it. Molecular switches are voltage-addressable, rather than field addressable. This is a major advantage in avoiding the half-select problem that can cause bits on the selected row but not the selected column to be written. Voltages can be much better controlled than field strengths.

We with our colleagues have previously reported molecular switches relying on electrochemistry to change from one state to another [3]. This experiment placed molecular-based configuration bits in a crossbar structure of singly configurable switches, each consisting of a single layer of rotaxane [4] molecules trapped between lithographically fabricated crossed wires. Measuring current flow at negative (reducing) voltage allowed the switches to be read. The switches could be irreversibly opened by applying a positive (oxidizing) voltage across the junction of the crossed wires.

These configuration bits are one molecule thick in the Z dimension, but they are about 10^4 molecules long in the X and Y dimensions. Since the functionality of a configuration bit is a property of a single molecule, the memories should in principle scale down to (a few) molecules per bit.

3. DEFECT-TOLERANCE

Chemically assembled molecular circuits will always have a small percentage of defective components because of the statistical nature of the assembly process. Chemical reactions have an imperfect yield. The resulting circuit

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will have uncertain connectivity. We have previously reported our strategy for using the reconfigurability of the architecture to work around these defects.

Our defect-tolerant strategy uses reconfiguration by first creating a special purpose computer to find defects, and then reconfiguring the system to avoid the defects and construct desired machine. We have successfully used this approach this approach in a machine built with conventional CMOS [5]. In the mid-1990s, HP Laboratories built a defect tolerant reconfigurable processor, Teramac, with 864 CMOS Field Programmable Gate Arrays. Teramac could be configured into many different types of special purpose computers, even in the presence of 220,000 defects. This is a defect tolerant, not a fault tolerant machine. By defect tolerance we mean the capability of a circuit to operate correctly without physically repairing or removing random defects incorporated in the system during manufacturing.

The crossbar structure can also be used to provide defect-tolerant configurable interconnect. The relative amount of resources devoted to interconnect and signal routing in any computer is huge compared to the number of resources devoted to logic, and for molecular scale electronics this imbalance will certainly grow even greater. The fat tree topology of Teramac consists of a set of crossbars, which are configurable to allow a vast choice of different paths to implement any logical circuit graph on the physical circuits of Teramac. By using crossbars consisting of crossed nanowires with molecules as the configuration bits that determine which wires are connected, we have a very efficient method for building a defect-tolerant interconnect. The fundamental reason that no one now uses FPGA-style configuration bits to create defect tolerant chips is that these memory bits are very expensive in a CMOS process. A configuration bit is about twenty times the area of the intersection of two minimal feature size wires, and thus the area utilized for defect tolerance can exceed that used for useful computation. In Teramac, 90% of the area was for configuration bits. This was reasonable in a research machine used to study multiple architectures, but it is not acceptable as a practical method of defect tolerance in CMOS integrated circuits. What makes defect tolerance practical in a machine using molecular electronics is that the molecules that are the configuration bits are much smaller than the area defined by the crossing of two nanowires. We build a configurable machine and get defect tolerance at essentially no extra cost.

4. LOGIC AND MEMORY

The objective of our crossbar architecture is to build integrated circuits, not just devices. This means that the molecular-electronics technology must be able to create logic and memory.

The work of Collier et al [3] demonstrated that this molecular-switch crossbar can be configured into a signal routing network, or, by addressing several crossbar junctions together, into either of two simple current-based logic gates (an AND and an OR gate). The molecular switches are only singly configurable, and so these molecular-based crossbars are not useful for Random Access Memory (RAM) applications.

This work demonstrates the ability to configure molecular crossbars into logic gates. All Boolean logic operations can be carried out with a minimum set of 3 logic elements: the AND gate, the OR gate, and the inverter. Of these three elements, AND and OR gates can be constructed from simple resistor networks, while the inverter requires a more complex physical realization.

Although the AND gate presented here is simply a resistor network, its response is much better than would be expected from standard resistors. Even if one had complete flexibility in choosing the values for the resistors in a standard network, the maximum difference one could hope for between the high and low states would be a factor of 2. However, we observe something closer to a factor of 15. This is because the current flow through our resistors is based on resonant tunneling through the rotaxane molecules, and so the resistance value of any given device is a strong function of the voltage that is dropped across the device. We present truth tables for an OR gate that was initially configured as a 3-input OR gate, but then reconfigured as a 2-input OR gate. Both versions of the OR gate yield quite high discrimination between low and high output states. The electronic configurability of these devices makes them extremely versatile, and the simplicity of the fabrication process makes them cheap to produce. Furthermore, the simplicity of these devices also makes it straightforward to quickly screen molecules for useful electronic properties. A challenge will be to scale down the size of the device, and integrate molecular switches with molecular-scale wires, such as metallic bucky tubes. The fact that the electronic properties of the rotaxanes are very similar in both the solid state devices and at the limit of a dilute solution of molecules, argues that these devices should scale down in size without much change in operation.

The same crossbar structure may be useful for performing arbitrary logic functions. If we form a diode crossbar (the molecular connections between the crossed nanowires act as diodes) the resulting circuit can also be used for computing arbitrary Boolean logic expressions given that the true and complement values of all inputs are both provided. This is because we can form wired ANDs followed by wired ORs. With these types of logic elements, it turns out that we can quite readily turn a 6x6 diode-crossbar into a defect-tolerant full 2-bit adder.

Our proposed cross-bar-based memory consists of two sets of overlapping nanowires, oriented perpendicularly to one another. Sandwiched between the wires are electrically addressable molecular switches. Electrochemical reduction or oxidation of the sandwiched molecule sets or resets the switches. A switch may be oxidized at one voltage, and its status may be read at a lower voltage. The voltages at which oxidation or reduction occurs are quite sharply defined. Reading at a lower voltage cannot reset the switch. When a switch is (electrically) closed, the resistance between connecting wires is low, and this constitutes a '1'. When the switch is opened, the resistance is high, and a '0' is stored.

There are several attractive aspects of this cross bar. We have previously reported chemically assembled periodic arrays of aligned nanometer scale wires [6]. Such arrays are very defect tolerant, both at the level of individual switches, and as an entire unit. Having a large number of identical units allows a defect tolerance procedure that depends on having large numbers of potential replacement parts available. This is a fine-grained architecture. At every junction there are several molecular switches. The switches are set by electrically biasing both a top and bottom wire, and carrying out a solid-state reduction or oxidation of the half dozen or so switch molecules that reside in the junction. This alters the tunneling resistance between the two wires and sets a memory bit.

5. CONCLUSIONS

One goal of a nanoscale technology is to provide many trillions of devices wired as a useful system. A self-assembling process is likely to produce only regular structures with low information content, but real computers built today have significant complexity imposed by human designers. A chemically assembled machine will have to be able to reproduce the arbitrary complexity demanded for general-purpose computation. This can be achieved within a crystalline network of wires and switches by being able to arbitrarily set any of the switches in an open or closed position, thus giving the capability of downloading or programming an arbitrarily complex circuit onto the regular but defective hardware platform. We have begun the first experiments to create such machines.

6. REFERENCES

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