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Molecular Nanoelectronics

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ABSTRACT

Both molecular switching and nanoscale wires have been recently demonstrated. We discuss their possible applications in circuits with emphasis on cross-point memories and programmable logic arrays.

1. INTRODUCTION

Reconfigurable architectures [1] are leading candidates for a technology to construct complex electronic circuits at the molecular scale. In turn, true molecular-scale electronics offer an ideal substrate for reconfigurable computing. The intrinsic strategies that we are presently using to create molecular scale electronics are very similar to those applied at a higher level of organization to construct reconfigurable computers.

All reconfigurable electronic circuits, such as Field Programmable Gate Arrays (FPGAs), are based on configuration bits. A configuration bit is, in essence, a memory bit controlling a switch. In CMOS technology, configuration bits are constructed from six or seven transistors. In a molecular electronics technology, a configuration bit could be a single molecule.

Our strategy is to use chemistry to create thermodynamically assembled devices that have a very simple arrangement, essentially a crystal. One then trains these 'self-assembled' crystals of devices to become complex programmed machines with a high degree of structure, which is downloaded after the device is assembled. The essence of doing this is to have a sufficiently fine-grained system with configuration bits that define the connectivity of the structure. This requires large numbers of molecular-scale configuration bits and wires. The fine granularity gives us considerable defect tolerance in the presence of a large number of configuration bits. If a part is defective and we can discover that it is defective, then we have enough connectivity and enough choices that we can route around it.

We present a strategy to create integrated electronic circuits manufactured from molecular-scale components [2]. The proposed technology is a collaboration of chemistry and computer science, allowing each discipline to do what it does best. We use chemistry to thermodynamically assemble regular but electronically useful structures at the nanometer scale. Then, we use computer science based computer aided design (CAD) algorithms to configure arbitrary electronic designs defined by opening and closing appropriate switches. Even though the chemically-assembled structures will be defective, the CAD algorithms are defect tolerant and the resulting integrated circuits are functional.

2. RECONFIGURABLE ELECTRONICS

2.1 Molecular Configuration Bits

In order to create a nanoelectronic configuration bit, we must have a molecular-scale memory that will open or close a switch, depending on the state of the memory. Such a device must operate at room temperature to be practical. We and our colleagues recently reported on the first potential molecular switches [3]. Molecular-based configuration bits were fabricated from a crossbar structure of singly configurable switches, each consisting of a monolayer of rotaxane [4] molecules sandwiched between lithographically fabricated metal electrodes. The switches were read by monitoring current flow at negative (reducing) voltage. In the 'closed' state, current flow is dominated by resonant tunneling through the electronic states of the rotaxanes. The switches were irreversibly opened by applying a positive (oxidizing) voltage across the device.

Molecular switches are voltage-addressable, rather than field addressable. In a CMOS based configurable device, two wires (address lines) are used 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.

The rotaxane molecular switch is irreversibly opened by applying an oxidizing voltage of +0.7 V or more. Once the switch has been opened, its status may again be read by applying a negative voltage. For an open switch, the measured current at –2 V is a factor of 50 to 100 less than that for a closed switch. The fact that calculations based on measured solution-phase electrochemical properties reproduced the properties of the solid-state devices provides further evidence that the switching is an intrinsic property of the molecule.

Although these configuration bits are one molecule thick in the Z dimension, they are 10^4 molecules long in the X and Y dimensions. But because the functionality of a configuration bit is a property of a single molecule, the memories should in principle scale down to (a few) molecular dimensions without appreciable loss of performance. When the molecular switches are closed, current flows through the switch via resonant tunneling through the molecular electronic states. The net result of this resonant tunneling is that the hi/lo current levels of the configuration switches are widely separated.

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2.2 Defect Tolerance

Any chemically-assembled molecular circuit will have a small percentage of defective components, if only because of the statistical nature of the assembly process. The problem is the imperfect yield of chemical reactions. The symmetry we expected to find in the structure will be broken by the defects. A fraction of the discrete devices will not be functional because of the statistical yields of the chemical syntheses used to make them. Because these components include wires, the system will suffer uncertainty in the connectivity of the devices. How can we be assured that it is performing error free computations? We have previously described a strategy for using the reconfigurability of our architectures to deal with these defects.

Our defect-tolerant strategy for utilizing molecular electronics takes advantage of reconfiguration by first creating a special purpose computer to find defects, and then reconfiguring the system to avoid the defects and construct desired machine. Having found the defects, we could create a special purpose machine to find the connectivity of the reconfigurable computer. We do not have to do this with the machines to be used by the final application. We can later reconfigure to handle the application defined by the end user.

We have confidence in this approach because it has been shown to work in conventional CMOS [5]. In the mid-1990s, HP Laboratories constructed an extremely defect tolerant reconfigurable processor, Teramac, out of 864 CMOS FPGAs. Because of the topology of the interconnection architecture chosen to implement powerful software algorithms, 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. We define defect tolerance as the capability of a circuit to operate as desired without physically repairing or removing random defects built into the system during the manufacturing process.

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.

3. 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.

3.1 Logic

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 portions of 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.

3.2 Memory

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. Because the molecular switches are designed to possess a large hysteresis in the voltammogram, a switch may be oxidized at one voltage, and its status may be read at another. 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 believe that periodic arrays of aligned wires will possible to chemically assemble because of their regularity. Such arrays are very defect tolerant, both at the level of individual switches, and as an entire unit. The large number of identical units makes possible a defect tolerance strategy that takes advantage of having large numbers of potential replacement parts available. This is a fine-grained architecture. At every junction there is not just one, but several (5 - 10) 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. The result of this process is that the tunneling resistance between the two wires is altered, and thus a memory bit is set.

4. SUMMARY

The traditional paradigm for computation is to design the computer, build it perfectly, compile the program, and then run the algorithm. The Teramac paradigm is to build the computer (imperfectly), find the defects, configure the resources with software, compile the program and then run. This new paradigm moves tasks that are difficult to do in hardware into software tasks.

One goal of a nanoscale technology is to provide a huge number (e.g. a mole) of devices for a system. A self-assembling process is only likely to produce fairly regular structures with low information content, but real computers built today have great 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.

5. REFERENCES

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