The Design of DNA Self-Assembled Computing Circuitry

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Abstract—We present a design methodology for a nanoscale selfassembling fabrication process that uses the specificity of DNA hybridization to guide the formation of electrical circuitry. Custom design software allows us to specify the function of a structure in a way similar to that used by VLSI circuit designers. In an analogous manner to generating masks for a photolithographic process, our software generates an assembly procedure including DNA sequence allocation. We have found that the number of unique DNA sequences needed to assemble a structure scales with its surface area. Using a simple face-serial assembly order we can specify an unambiguous assembly sequence for a structure of any size with only 15 unique DNA sequences.

Index Terms—Associative memories, computer architecture, DNA self-assembly, nanoelectronics, parallel processing.

I. INTRODUCTION

C OMPUTER system design will change dramatically as nanoscale science and technology are developed to the point where practical assembly mechanisms exist for building large-scale systems. These changes will be motivated by emerging capabilities and an interest in developing early-term computing devices that can exploit the technology's features. The advent of massively parallel near-molecular scale electronic systems will open wide problem spaces yet untouched by modern computing [1].

We focus on the realization of a new computer architecture that is enabled by the development of DNA-guided self-assembled systems. The enormous parallelism and scale of this kind of self-assembling process has motivated research into novel forms of computation that use the intrinsic properties of DNA hybridization to form solutions to a problem [2], [3]. We have considered a slightly different approach to developing computing devices using DNA. Instead of depending on the computability of DNA hybridization events we investigate the structural use of DNA to create electrically active nanoscale rod-lattice structures. These structures can then be used in the designs of computing circuits that solve particular classes of problems. Later, we discuss a class of problems and a computer architecture to which this form of self assembly is suited.

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In brief, we envision a machine fabricated by the DNA-guided self-assembly of silicon nanorods. The self-assembly is guided by the thermodynamic properties of DNA that give it a unique ability to form pairs among complementary strands. The DNA guides the placement of semiconducting, conducting, and insulating rods to form a three-dimensional (3-D) structure that implements a CMOS circuit. The large-scale synthesis benefits of self assembly (e.g., on the order of 10^{19} assembly events in parallel) could make this technique a powerful alternative to photolithography.

II. BACKGROUND

Our method of constructing computing circuitry from nanoscale self-assembled components appears to require several capabilities that we describe here. These capabilities, described below, include the functionalization of rod-like nanowires with DNA, DNA metallization, DNA-guided self-assembly, and the simulation of nanoscale transistors.

Nanowire DNA functionalization is the first step to implementing a DNA-guided self-assembly process. Our method requires the rod-like nanowires to have unique DNA attached to each end. Later, we will discuss how to design the DNA and nanowire properties to assemble computing circuitry. The DNA-directed formation of nanowire-patterned surfaces has been reported and provides insight into how such nanowires can be functionalized [4].

The ability to convert double stranded DNA into a highly conductive ohmic contact by a metallization process makes the use of DNA in nanoscale circuitry extremely attractive [5], [6]. This also alleviates the difficulty of using the native insulating properties of untreated DNA [7]. Further, such metallization techniques are suitable for either surface bound or suspended DNA strands. We anticipate that the DNA used to form our 3-D self-assembled structures will exist in a suspended form similar to what has been reported [5].

An important quality of DNA that makes it most suitable for self-assembly is its ability to hybridize with its complement with very high specificity. Consider the 4^8 different 8 base DNA sequences, there are 65 536 *nearly* orthogonal reactivities. This is a vast improvement over the handful of specific covalent chemical reaction schemes that are readily accessible today without using DNA (or RNA) binding methods [8].

Remarkable work has been undertaken in the effort to produce DNA assembled structures. Many of these efforts have focused on the structures created by clever designs of DNA sequences undergoing interesting thermodynamic transitions [9], [10]. Still others have focused on the formation of ordered superlattices



Fig. 1. The basic structure of the ring-gated field-effect-transistor.



1 micron

Fig. 2. A scanning electron microscope image of AuPd rods projecting out of a poly-methyl-methacrylate (PMMA) surface.

made from nanorods [4], [11]. The experimental demonstration of mesoscopic DNA-guided assemblies is also of interest [12]. These results imply that there is considerable promise in the DNA-guided self-assembly of large-scale molecular structures.

Controlled self-assembly of nanoscale circuitry requires the ability to control the properties of individual components of the structure. Recent advances in silicon nanowire doping have proven that small nanoscale rods can be doped controllably and can be made to behave like bulk semiconducting materials [13]. These results have encouraged us to explore the use of semiconducting (n-type and p-type), metallic, and insulating nanowires within the larger context of computer circuit fabrication, design, and simulation.

Accordingly, we have evaluated a new kind of transistor that we call a ring-gated field effect transistor (RG-FET). Fig. 1 illustrates the basic structure of the RG-FET. The ends of the rod are the source/drain contacts and the band around the middle of the rod is the gate. We have simulated the behavior of this kind of transistor in CMOS logic circuits [14], [15]. We have also briefly explored the plausibility of fabricating such a transistor by using an electron beam lithography technique to form a nanoporous polymer surface. Fig. 2 is a scanning



Porous alumina / polymer membrane

Fig. 3. RG-FET synthesis scheme. Repeated membrane etching and rod surface treatments for the structure.

electron microscope image of AuPd rods projecting out of a poly-methyl-methacrylate (PMMA) surface. The route that we expect will most likely lead to successful patterning of the rods is illustrated in Fig. 3.

The process begins by forming rods in a membrane (either ceramic or polymer) and using a selective etch to expose a portion of the rods. Using silane, polymer, or other resists, the top portion of the rods could be modified and protected from subsequent etching steps. A negatively charged silane monolayer could then be used to form a band around the rod that could be processed to create a metallic ring as reported by Richter [6]. A strand of DNA could then be attached to the ring to allow a gate electrode to connect later.

III. ASSEMBLY METHOD

We are interested in developing computing devices from self-assembled structures. Our proposed method employs the assembly of simple cubic unit cells (with diagonal supports) using DNA-guided self-assembly for use in electrical circuitry. Control over the electrical properties of the assembled structure comes from choosing the electrical properties of the individual rods used to form the structure. For this purpose, we have developed custom software to allow a circuit designer to layout the 3-D structure of a logic gate. The software automatically generates a list of rod types and the DNA sequences required on each end given the 3-D specification of the structure. First, it is important to understand our proposed assembly process before examining the algorithms used in the design software. As an example of the assembly process, let us consider the assembly of a simple three-rod, triangular structure.

Fig. 4 illustrates the steps involved in the process. The process begins by 1) hybridizing a rod with the solid support (or anchor). The rod, which is normally incompatible with aqueous reactions, can be solublized by the use of a low concentration of surfactant and constant agitation. Such treatments are commonly used to prevent stiction in microelectromechanical systems (MEMS) and other silicon self-assembly schemes [13], [14]. The solid support, typically polystyrene or silica microspheres, has been previously functionalized with a strand of DNA that has two regions. The first rod of the assembly has DNA on one end that is complementary to the first region of DNA on the solid support. The DNA sequences attached to the solid support are extended away from the surface by a polymer arm that has a sufficiently negative linear charge to metallize, as





Fig. 5. Cubic unit cell with diagonal supports. The light gray rods are conducting and the dark gray rods are insulating.

Fig. 4. Assembly of a triangular rod structure.

does DNA [5], [6]. It is important to control the density of the polymer arm in order to prevent structures from interfering with each during the assembly process. The solid support is used to anchor the intermediate structures during the cycling of reactants and rods.

The hybridization event between the first rod and the solid support is carefully controlled to maximize the specificity of the interaction. By raising the temperature of the system above the melting temperature of the DNA and then slowly cooling it back to room temperature, we can expect a high degree of specificity between the DNA strands (i.e., complementary strands hybridizing with each other, and each other only). Nonspecific rod–rod interactions may interfere with this intended interaction without further treatment. The experimental determination of an appropriate concentration of surfactant may alleviate this trouble.

After the hybridization event, the duplex DNA is crosslinked using cisplatin or some other crosslinking agent (step 2 in Fig. 4). In general, each hybridization event is carried out under these same conditions to maximize specificity. This is important for driving the assembly to completion with high fidelity (for high yield). One particular study places the DNA hybridization efficiency of a 12-base pair strand with its complement at around 98% [18]. This is a considerably lower yield per device than conventional CMOS (~99.999 99%) and will demand a defect tolerant architecture to be useful [19], [20].

The second rod, which has complementary DNA on one end to the second region of DNA on the solid support, is flushed past the solid support, and under the same stringent conditions, allowed to hybridize with the solid support (step 3). Again, the duplex DNA is crosslinked to form a stable and covalently bound intermediate structure (step 4).

Unfortunately, the addition of the third rod is not as simple as the previous two. If we were to add a third rod that had DNA on each end that was complementary to both the first and second rod, we could form a triangular structure. But we would also form a four-rod structure with relatively high probability. This is because the third rod could hybridize independently with both the first and second rods. To avoid this ambiguity we need to introduce a "coupling" DNA strand.

The third rod is made so that it is complementary on one end to only the first rod. The other end of the third rod is made to complement one side of the coupling strand. The third rod is hybridized with the first rod as described earlier (steps 5 and 6). The coupling strand is made to complement the free end of the third rod and the free end of the second rod, with one modification. The portion of the coupling strand that hybridizes with the third rod has a psoralen-modified nucleotide, or some other site-specific mutagen. This modification ensures that the coupling strand irreversibly binds only to the free end of the third rod.

The coupling strand is hybridized with the third rod, as before (step 7). If the site-specific mutagen requires any special processing, that processing is performed now. After the coupling strand has been bound to the third rod irreversibly, the system's temperature is raised above the melting temperature of the coupling strand and rinsed with buffer. Upon cooling, the coupling strand that was bound to the third rod will hybridize with the second rod. This unambiguously closes the gap and forms the triangular structure. Crosslinking the duplex DNA, again, will form a covalently bound and stable structure (step 8). Metallization can occur anytime after the structure has been formed [5], [6].

A. Cubic Unit Cell Assembly

Fig. 5 illustrates a simple cubic unit cell with diagonal supports. The particular function of any unit cell is determined by the electrical properties of each rod. By using the RG-FETs and rods described earlier, the cell can be combined with other cells to form logic circuitry.

The logic circuitry is first specified using a CMOS logic style, as in Fig. 6. The NAND gate shown in Fig. 6 takes its two inputs, A and B, and produces an output of zero if and only if the two are both one ($V_{\rm dd}$). This logic gate represents one of many complete logic sets because groups of NAND gates can be used to implement any Boolean logic function.

The circuitry of the NAND gate can be converted into a suitable 3-D structure, illustrated in Figs. 7 and 8, for self-assembly. The procedure described earlier for the formation of a triangular structure can be extended to form such a rectangular solid as this logic gate. Instead of using a single type of rod, the NAND gate will require each rod to be one of the four rod types (n-type or p-type semiconductor, metallic, or insulating) described earlier. Conducting rods can be attached to the metallic gate of each RG-FET by hybridizing with the DNA strands on the ring and a corner of the cubic unit cell.

One challenge is that the number of unique DNA sequences that this method requires scales with the surface area of the structure. Fortunately, it is possible to conserve the number of unique DNA sequences required to assemble a structure by using a face-serial approach. This is important since the number of unique DNA sequences needed by even a simple memory element (256 bits) could easily reach tens of thousands.



Fig. 6. CMOS implementation of a NAND gate.



Fig. 7. Conducting portions of the 3-D structure for a NAND gate. The rods with bands around their middles are semiconducting (n-type or p-type.).



Fig. 8. Physical 3-D structure of a NAND gate embedded in insulating unit cells for structural support.

In this approach, each face of the structure is assembled in a serial fashion. Since each face is assembled independently, faces can each share a common set of "active" DNA sequences. Within a face, the assembly moves from left-to-right, top-to-bottom. Fig. 9 illustrates the assembly sequence. Since a common set of DNA sequences is shared between faces as well as between sites within a face, the total number of unique DNA sequences is fixed and independent of the surface area of the structure. Our designs use 15 unique DNA sequences for this face-serial method. Table I contains the counts of our assembly method for several logic circuits. Fig. 10 illustrates the NAND structure as viewed when each unique DNA strand is given its own color (or shade of gray.) The repetition among rows on each face is apparent and indicates that the total number of unique DNA strands is fixed.



Fig. 9. Face-serial assembly of a 3-D structure. (partially completed in this figure).



Fig. 10. Three-dimensional structure of a NAND gate with each unique DNA allocation represented by a different color (shade of gray).

The statistics for Table I came from a custom assembly tool that we have developed for converting 3-D circuit specifications into rod-DNA allocations. These statistics indicate that as the logic circuitry becomes more complex, so does the number of required unique DNA sequences. This underscores the importance of the DNA conserving, face-serial assembly method described above.

B. Power and Input/Output Connections

The problem of connecting the self-assembled structures to power and I/O electrodes is important because it could easily become the manufacturing bottleneck given the vast number of structures that can be assembled at one time. Therefore, we need an easily implemented interconnection method that works for vast numbers of devices in parallel. Further, the method must be useful for connecting structures that either may be deposited from a suspension or be grown in situ on a metallic surface.

Our solution is to create a vertically layered system with self-assembled structures sandwiched between two power electrodes. Fig. 11 illustrates the idea. Each electrode serves a dual purpose. The bottom electrode (P_0) is used to electrically ground the circuitry and is also used as a clock signal. The top electrode (P_1) is used to supply a positive voltage to the circuitry and is also used as a data signal.

This arrangement requires special "power-up" circuitry to be embedded into the structures for them to function properly. The power-up circuitry serves to orient the structure as to which direction is "up" (the positive voltage electrode). This same circuitry, through the use of a bridge rectifier, can supply power and provide a reference for how to use each electrode. By alternating between power and signaling phases, the electrodes

Logic Gate	Total Rods	Metallic	Insulating	Struts	RG-FETs (& gates)	DNA Sequences*
NOT	90	5	47	34	2	26
NOR	252	18	122	104	4	55
NAND	328	18	164	138	4	63
XOR	522	86	190	214	16	77
Full Adder	1722	273	641	732	38	158

TABLE I Assembly Statistics for Several Logic Circuits

* The number of DNA sequences needed if the conserving allocation method is not used. The conserving allocation method needs 15 unique sequences.



Fig. 11. Layered interconnect method. The bottom electrode serves as ground while the top electrode serves as $V_{\rm dd}.$

can be used for both purposes. The initialization routine for this system is as follows.

- 1) The positive electrode (P_1 in Fig. 12) is slowly ramped to V_{dd} (1 V in the circuits we have considered) and the ground electrode (P_0 in Fig. 12) is connected to the system ground (0 V).
- 2) After some time the orientation capacitors (C_{or0} and C_{or1}) will have fully charged or failed to charge depending on which electrode was powered-up and which was grounded. At this point the power-up circuit "knows" which electrode (P_0 or P_1) is the positive (and data) electrode and which is the ground (and clock) electrode. The signals F_0 and F_1 will reflect this orientation and select the proper electrode to be connected to the internal DATA and CLOCK wiring.
- 3) At this point binary I/O can occur. To signal a "1," the positive electrode and ground electrodes are temporarily held high. The ground electrode is returned to ground potential after the circuitry has stored the input bit. To signal a "0," first the positive electrode is grounded and then the ground electrode is raised to V_{dd} . Again, this condition is maintained for a sufficient time to allow the circuitry to latch the input bit before returning to the power phase (P₁ high and P₀ grounded).

The bridge rectifier in the power circuitry charges a capacitor (and the rest of the power-up circuitry) regardless of which electrode is positive. The circuitry will function properly as long as the data and clock steps (step 3 above) are quick in comparison to the power-up time constant (i.e, the time required to charge the power circuitry).

This circuitry is useful because it works without regard to which electrode is positive and which is grounded. If the assembled structures are to be deposited from suspension, they should be encased in a way similar to that illustrated in Fig. 13.

This structure connects opposing sides of a cube (or rectangular solid) to the P_0 and P_1 wiring inside the structure. Since each side of the cube is connected either to P_0 or P_1 , the struc-







Fig. 13. Symmetric structure able to land on any face and connect two internal nodes.

ture can land on a metallic surface (the bottom electrode) with any of its sides. A layer of insulating material (e.g., a polymer) could be deposited onto the surface and etched back to expose the upward side of each cube. Another layer of metal could then be deposited on top and used as the positive electrode. This method can be used regardless of how the cube lands as long as it makes (or can be made to make) good ohmic contact with the bottom and top electrodes.

IV. COMPUTER ARCHITECTURE

The early limitations of a self-assembling realization technology will require small circuitry. Single bit, serial processing elements are well suited to such limitations. They require less circuitry and have simple interfacing requirements. En masse, such processing elements can perform incredible computational feats. Consider distributed computing projects like "SETI @ home" and the "United Devices Cancer Project" that use massive parallelism to accomplish super-computer scale tasks with idle desktop computer processing cycles.

In the following section, we briefly discuss a type of architecture that can take advantage of the features that our self-assembling technique has to offer. In many respects, this architecture is uniquely enabled by the technology.

A. Decoupled Array Multi-Processor

A decoupled array multiprocessor is a large collection of simple processing elements similar to a CM-2 but without the rich interconnection fabric between elements. Each processing element, of which there are approximately 10^{12} , has a built-in random number between 0 and 240 formed during the self-assembly process. This random number is used by a parallel program, run by all the processing elements at once, to perform a unique set of operations on data that is broadcast to all elements. In this way each processing element can perform a set of operations determined by its random number. For example, instructing each processing element to divide a global number by its random number and checking for a remainder would test the global number for primes. Any processing element that finds no remainder during the division will elect to notify the user that its random number divides the number under test. It is a simple matter to find prime numbers this way.

Architecturally, there are two ways to interact with the processing elements of the decoupled array multiprocessor. The elements will 1) perform basic arithmetic operations (including register transfers and conditionals) and 2) respond to simple queries.

B. Optimization Problems

The decoupled array multiprocessor can be applied to nonlinear problems that have no simple, conventional solutions. In the prime number example above, each processing element performs a division using its random number and compares the remainder with zero. If the remainder is not zero, the processing element sits quietly and will not respond to any queries. If the remainder is zero then the processing element communicates with the outside world (because it has a factor!). In contrast, an optimization program would perform a comparison with a reference number before communicating with the outside world.

In this scenario, each processing element compares its arithmetic result with a number broadcast to all elements. A minimization program will only respond to the query if the element's result is less than the broadcast number. A maximization program will only respond to a query if the element's result is greater than the broadcast number.

This method of selectively controlling a large population of processing elements reduces communication bandwidth and distributes the computation among eligible processing elements, which can help to reduce power consumption.

V. PRACTICAL OBSTACLES

The fabrication technique described here relies heavily on experimental processes that are only beginning to be understood. There are several crucial issues that need to be resolved before the discussion of DNA-guided self-assembly can mature. The following is a list of a few of these problems.

- Finely controlled synthesis of doped silicon nanorods: Experimental results have demonstrated that it is possible to use doped silicon nanorods in CMOS circuitry. However, tight control over the distribution of nanorod lengths (not just diameter) is required for an efficient assembly process.
- 2) Asymmetric nanorod functionalization: The attachment of two differing sequences of DNA to a nanorod is the fundamental property of this assembly technique that enables the fabrication of complex aperiodic structures.
- Reduction of nonspecific nanorod binding: The self-assembly of nanoscale components is hindered by surface area effects that limit the yield of the process. Such nonspecific interaction must be minimized to enhance specific (e.g., DNA binding) assembly events.

VI. CONCLUSION

We have presented a method for the DNA-guided self-assembly of cubic unit cells that is suitable for fabricating computing circuitry. Our custom design software enables us to specify 3-D structures that implement logic gates and generate an assembly procedure based on the structure. We have developed an algorithm that assembles structures in a face-serial method that requires only 15 unique DNA sequences.

Computer architecture will undoubtedly reflect the dramatic achievements being made in nanoscale science and engineering. For the near term, we have presented a computer architecture that can take advantage of a low bandwidth, single-port communication channel by using a massively parallel set of independent processing elements.

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