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Modeling and simulation of a nanoscale optical computing system

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HIGHLIGHTS

- We propose a method to build computing systems with nanoscale optical devices.
- An Optical Logic Element (OLE) is proposed as a basic compute unit.
- We demonstrate optical coupling between optical fibers and chromophores.
- We build and validate a SPICE model for OLEs, and analyze various logic circuits.
- OLE power-delay product is 2.5× lower and area density is 100× higher than CMOS.

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ABSTRACT

Optical nanoscale computing is one promising alternative to the CMOS process. In this paper we explore the application of Resonance Energy Transfer (RET) logic to common digital circuits. We propose an Optical Logic Element (OLE) as a basic unit from which larger systems can be built. An OLE is a layered structure that works similar to a lookup table but instead uses wavelength division multiplexing for its inputs and output. Waveguides provide a convenient mechanism to connect multiple OLEs into large circuits. We build a SPICE model from first principles for each component to estimate the timing and power behavior of the OLE system. We analyze various logic circuits and the simulation results show that the components are theoretically correct and that the models faithfully reproduce the fundamental phenomena; the power-delay product of OLE systems is at least 2.5× less than the 14 nm CMOS technology with 100× better density.

1. Introduction

The well-established scaling challenges that CMOS faces as feature sizes approach tens of nanometers have motivated research into alternative technologies for more than a decade. However, despite advances in next-generation transistor designs and foundry processes, power efficiency and thermal budgets continue to dominate the performance envelope of current systems.

Among the disruptive technology candidates that might one day supplement CMOS, the self-assembly of DNA into nanoscale logic circuits is a promising scheme. DNA can form structures with molecular precision, i.e., sub-nanometer, over several square microns and with massive assembly parallelism, e.g., $>10^{15}$ structures, in only a few hours of processing. A remaining challenge is to pattern useful building blocks on the DNA nanostructures to compose larger systems.

Molecular-scale computational devices have been patterned on DNA self-assembled grids and can be used to create simple logic circuits and computing systems [25,27]. Further, a variety of logic functions have been demonstrated including simple logic gates, combinational and sequential gate arrays with molecular devices [28]. However, the physical integration of molecular logic gates into serial cascades remains a problem because they often use incompatible inputs and outputs to represent binary signals.

In this paper, we demonstrate a method of integrating small molecules called chromophores into Resonance Energy Transfer (RET) logic gates on DNA nanostructures to build computing systems interconnected by optical waveguides, e.g., optical fibers. Similar to wavelength division multiplexing (WDM) input and

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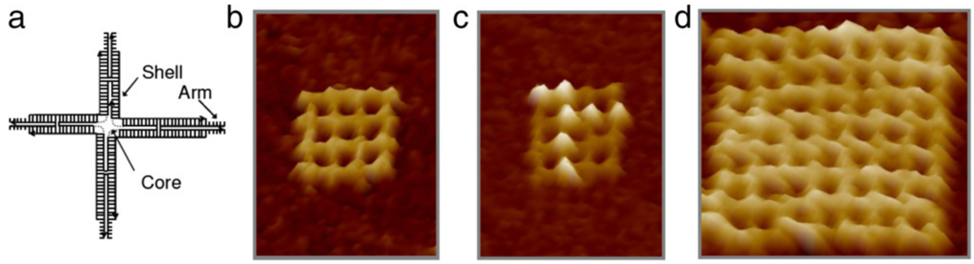


Fig. 1. (a) Cruciform motif and Atomic Force Microscopy (AFM) images of: (b) a 60 nm × 60 nm DNA grid, (c) a grid with a pattern of single molecules, and (d) a 140 nm × 140 nm grid.

output signals in this system are represented by the presence (i.e., true) or absence (i.e., false) of a set of optical frequencies. We design an Optical Logic Element (OLE) as a basic unit from which larger systems can be built. An OLE is a microscale layered structure that works similar to a five-input lookup table (5-LUT) common in FPGAs, but instead uses wavelength division multiplexing for its inputs and output. An OLE has three basic components: (1) input and output color filters to select target wavelengths, (2) a non-linear gain media, such as a layer of quantum dots, and (3) DNA self-assembled minterms implemented with RET logic. Optical fibers can be used as wires to interconnect OLEs into larger systems as a surrogate for microscale patterned waveguides currently used to create on-chip optical networks.

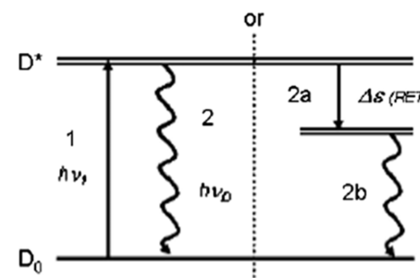
To demonstrate this scheme, we build a SPICE model from first principles for each component to estimate the timing and power behavior of an OLE and fiber. We analyze various logic circuits, e.g., a 2-input multiplexer, 1 bit full adder, an oscillator, a D-F/F, a carry-lookahead adder, etc. to understand their behaviors and design requirements for an experimental demonstration. Eventually, the SPICE model output will serve as a set of technology parameters for a larger-scale system simulation framework to evaluate architectural designs.

The simulation results show that the components are theoretically correct and that the models are self-consistent and faithfully reproduce the fundamental phenomena from which they were built. We also apply a power model for the OLE to show that the power-delay product (PDP) of those circuits is at least 2.5× less than that in state-of-art CMOS technology with at least two orders of magnitude better area density.

The rest of the paper is organized as follows: Section 2 describes DNA self-assembly and RET logic circuits. Section 3 introduces our system for optical computing including the OLE structure. Section 4 presents the details of the SPICE model for OLEs. Simulation results and analysis for a set of common logic blocks are shown in Section 5 and we conclude in Section 6.

2. Background and motivation

The OLE is the basic building block for the proposed system and is built from components that can be fabricated by conventional lithographic techniques with the exception of the logic minterms which we synthesize by DNA self-assembly. We have previously shown how DNA self-assembly can be used to build ultra-dense optical logic gates, e.g., 2 nm × 2 nm × 2 nm two-input AND gates [27], however, these structures are not easily interconnected into larger systems. In order to create a scalable logic system from self-assembled gates, we begin to investigate feedback and gain mechanisms as well as optical interconnection at micron scales to make hybrid micro–nano systems in the laboratory. In this section we provide a brief background on DNA self-assembly, RET logic, feedback and non-linear gain media and optical interconnection which motivate us to create the OLE and its SPICE model, and to evaluate more complex logic functions.



$$D + A \xrightarrow{h\upsilon_1} D^* + A \xrightarrow{RET} D + A^* \longrightarrow D + A + h\upsilon_2$$

Fig. 2. Transition diagram of RET.

2.1. DNA self-assembly

DNA self-assembly is a bottom-up fabrication technique with sub-nm precision that can organize single-molecules into complex and arbitrary patterns. Self-assembly is a spontaneous reaction among strands of DNA that can be controlled by careful sequence design. The entire process is highly scalable and leverages industrial synthetic chemistry which has an infrastructural base the rival of the entire semiconductor industry. In this way, a specific topology of molecules can be created with inter-molecular distances with sub-nm resolution and enormous manufacturing scales (i.e., $>10^{15}$ structures/hour). Fig. 1 illustrates the DNA grid we use as a substrate for RET logic. The motif shown in Fig. 1(a) is composed from nine strands of DNA: one core, four shell, and four arm strands. Grids can be formed by mixing motifs with arm sequences designed to organize finite, square lattices as shown in Fig. 1(b)–(d). Precise chemical patterns, Fig. 1(c), can be made by modifying select motifs, e.g., by modifying one of the nine DNA strands, prior to assembly into a lattice. DNA grids can implement energy transfer circuits that function similar to diode–diode logic by organizing chromophores into geometric patterns. Chromophores are small molecules that absorb light at one wavelength and emit at a different lower energy wavelength [21]. The next section describes the underlying resonance energy transfer phenomena, and how to build RET logic.

2.2. RET logic

In this section, we introduce the basic process used in our proposed system to perform computing—Resonance Energy Transfer (RET). First, we describe the details of the RET process and how it can be used to construct logic gates. Next, we demonstrate a RET logic gate we fabricate in a lab environment. Then we compare the area density of RET logic gates with the state-of-the-art CMOS process.

2.2.1. Resonance energy transfer

Resonance energy transfer is the foundation for the logic circuits in the proposed system. Fig. 2 illustrates the RET process that occurs between a donor, which is excited either electrically