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Modeling and Simulation of DNA Origami based Electronic Read-only Memory

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***Abstract*— Deoxyribonucleic acid (DNA) has emerged as a promising building block for designing next-generation ultra-high density storage devices. Although DNA is highly durable and extremely high density in nature, its potential as the basis of storage devices is currently hindered by limitations such as expensive and complex fabrication processes and time-consuming read-write operations. In this article, we propose the use of a DNA crossbar array architecture for an electrically-readable Read-Only Memory (DNA-ROM). For DNA-ROM, we have chosen two DNA strands for representing Bit 1 and Bit 0 respectively. DNA charge transport has been studied through a 'contact-DNA-contact' setup. The results obtained from the DNA charge transport study have been used to analyze the crossbar array. The performance has been analyzed by loading an image onto a 128×128 crossbar. For this application, we have observed a bit error rate of 4.52% and power consumption of 6.75 µW.**

Keywords*— *Deoxyribose Nucleic Acid (DNA), Nanoelectronics, Memory Storage

I. Introduction

Production of digital data is increasing exponentially [1], driven predominantly by the adoption of artificial intelligence (AI) and deep learning. According to current projections [2], approximately 175 zettabytes (10^9 terabytes) of new data will be generated annually by 2025. Archival storage of even a fraction of such immense data requires a fundamental rethink in durable, low power, accurate, and extreme high-density storage technology since traditional storage devices (e.g., magnetic tapes, hard disks, Blu-ray, and solid-state devices) are fast approaching their scaling and performance limits and further downscaling of such devices will result in performance degradation. This motivates the demand for the development of alternate ultra-high-density storage technologies which are durable and energy-efficient.

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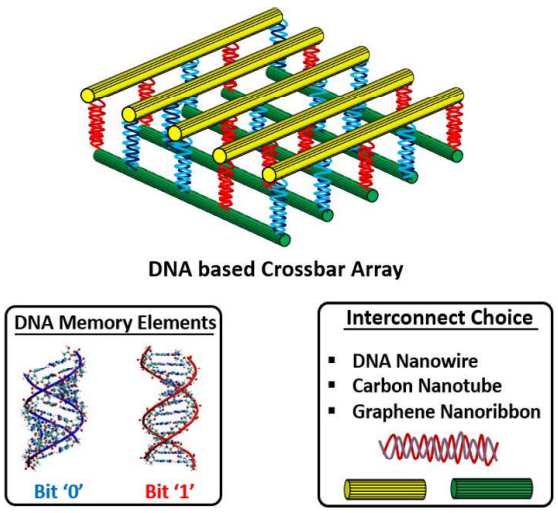

Fig.1. Conceptual illustration of a DNA crossbar array. DNA origami forms long DNA nanowires as interconnects and short DNA sequences as memory cells. These components can be self-assembled to create a crossbar like architecture. An electrical read-out mechanism can be adopted for retrieving the information in the DNA crossbar array.

Deoxyribonucleic acid (DNA) is one of the most promising candidates for high-density storage devices. The concept of using DNA for data storage dates back to the mid-1960s when the idea of 'genetic memory' was proposed by Neiman and Wiener. However, technological limitations at the time concerning DNA sequencing and synthesis limited the practical viability of such memory devices. Around 1986, Davis *et al* [3] and Clelland *et al* [4] made the first experimental demonstrations of DNA storage. Other noteworthy activities

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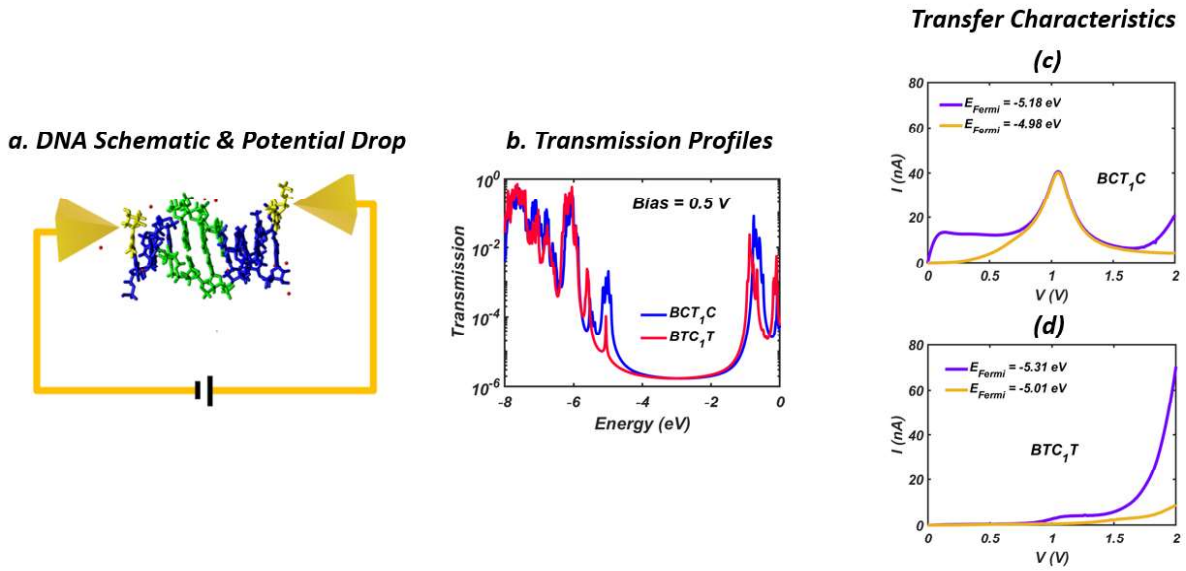

Fig.2. (a) DNA between two metal electrodes connected to a battery. A DNA molecule is placed between two electrodes and a voltage bias is applied across it. For our work, two double strand DNA sequences with B-conformation are considered, $C_3T_1C_3$ and $T_3C_1T_3$ ($C_3T_1C_3$ refers to the sequence 3'-CCCTCCC-5'). (b) Transmission profiles for CT_1C and TC_1T B-DNA sequences as a function of energy (δ) at an applied bias of 0.5 V. Transfer characteristics for (c) CT_1C and (d) TC_1T B-DNA sequences at two different Fermi energy levels.

include the works referenced in [5]–[12]. A breakthrough was achieved in 2012 when Church *et al*. [13] first demonstrated the concept by successfully storing hundreds of kilobytes of data. Independent observations made around the same time by Goldman *et al*. [14] further validated the viability of DNA digital storage. This paper does not address this line of prior work. Instead, it proposes an electrically-readable memory array idea based on DNA Origami.

The rest of the paper is structured as follows. The concept of DNA-ROM is presented in Section II. The method for calculating current flow in DNA is addressed in Section III, which is followed by a discussion of the performance analysis of a DNA-ROM array in Section IV. We conclude this paper with a brief discussion of ongoing and future work in Section V.

II. DNA-ROM CONCEPT

Even though DNA-based storage systems have the potential to be a transformative technology for next-generation storage applications, it is still at their nascent stages [14], [15]. In this paper, we address the random access and read latency issues by adopting a crossbar array architecture for an electrically readable Read-Only Memory (ROM) device [16]. Some advantages of crossbar architectures are non-blocking input/output signal flow, fabrication simplicity, and high density [17]–[19]. Our proposed device is composed of interconnects and two different DNA sequences serving as memory cells, as illustrated in Fig. 1. In contrast to existing DNA-in-solution storage systems where bit strings are encoded into a DNA sequence, we choose an "appropriate" pair of DNA sequences and exploit the difference between their "characteristic conductance" to reliably store binary information. Motivated by recent advances in the field of synthetic biology, we propose the self-assembly of crossbar nanostructures using DNA origami-inspired approaches [20], [21]. From a fabrication perspective, our scheme leverages synthetic biology approaches for fabricating and programming memory cells but requires conventional semiconductor and lithography processes to enable electrical read-out. Instead of top-down lithography, advances in DNA technology are to be considered for the realization of this technology. Random access is ensured by the correct selection of voltage lines (wordlines & bitlines) in the crossbar array during the read-out process. While electrical read-out is well studied in the context of other crossbars (e.g., RRAM) arrays, ensuring proper electrical contacts can be challenging in a microfluidic environment.

III. DNA CHARGE TRANSPORT

We study charge transport through a 'contact-DNA-contact' setup as illustrated in Fig. 2a. We employ a combination of density functional theory (DFT) and charge transport calculations to generate the current-voltage characteristics of the DNA strands' (CT_1C and TC_1T B-DNA). First, we generate the DNA strands and minimize the energy of the structures in the solution (water + counterions). Next, we use the energy-minimized structure as input for the DFT step. Here, we only include the DNA strand and the closest counterions to the DNA to neutralize the DNA molecule and employ the polarizable continuum model to account for the solvent dielectric effect.

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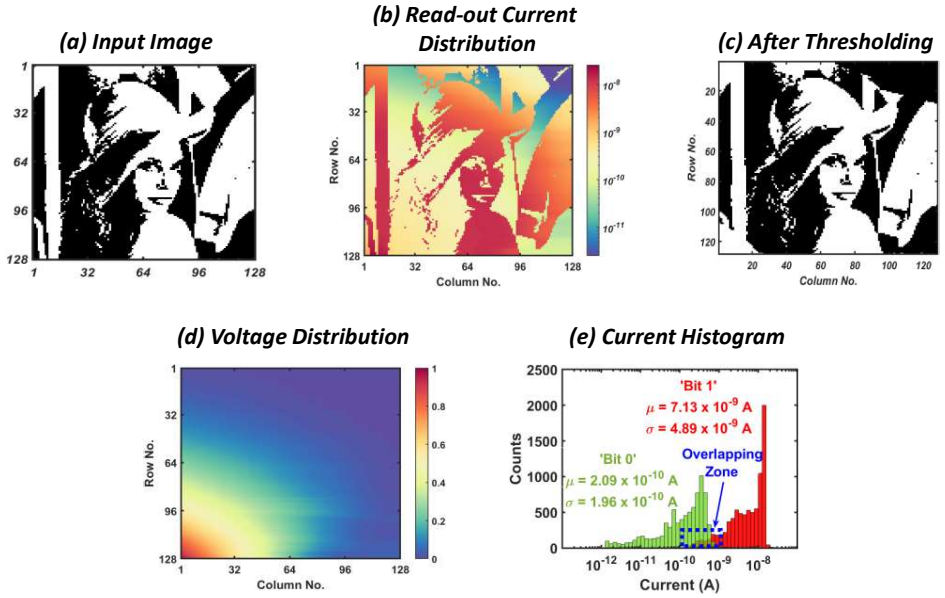

Fig.3. Crossbar simulation results: (a) the input 'Lena' image, (b) the read-out current distribution after crossbar simulation (the color bar on the right represents current in amperes), (c) the final image read after thresholding, (d) Voltage distribution across the crossbar, (e) Histogram showing the overlap zone between Bit '1' and Bit '0' current distributions which leads to bit error.

The DFT calculations yield the system Hamiltonian which describes the energy levels of the DNA and their electronic coupling. We then use the Hamiltonian as input for charge transport calculations using Green's function with Büttiker probes to account for decoherence. The output from the last step yields the electron transmission profiles and the current-voltage characteristics shown in Figs. 2b, 2c, and 2d. In calculating the charge transport, we assume that contacts are made at the two ends of the strand (3' and 5' ends). Computation of the potential drop across the molecule requires self-consistent calculations that account for contact details (geometry of atoms and bonding to DNA) and appropriate boundary conditions for solving Poisson's equation [22]. These requirements are difficult to achieve in a DFT-based calculation for a molecule of several hundred atoms. Therefore, our approach is to assume a potential drop profile *a priori* and apply it to charge transport calculations. Further details of DFT and charge transport simulations can be found in our previous work [23]. We assume a nonlinear voltage drop occurring in the DNA: 40% of the voltage drop across each of the two contact points, and the remaining 20% drop linearly along the rest of the DNA strand. It has been observed that if the applied bias is in the range [0, 1] V, the currents of these two strands differ by about an order of 2. This makes these two strands suitable for representing Bit '1' and '0' memory states in the proposed DNA-ROM technology.

IV. DNA-ROM Simulation Results

From the DNA transport simulations, we have created a look-up table for calculating DNA currents at various voltages during crossbar simulation. Since the current-voltage characteristics for both DNA strands are nonlinear, as can be seen in Figs. 2c and 2d, we have adopted an iterative approach for computing the voltage distribution across the crossbar. The iterative process commences with a small applied voltage of 0.05 V to obtain the initial conductance matrix by interpolating from the look-up table. Based on the conductance values of DNA memory cells, the voltage distribution in the array is calculated using the following equation:

$$V_{ij} = \frac{1 + \sum_{k=j+1}^{n}\left(G_{ik} * \sum_{l=j+1}^{k}\frac{1}{g_l}\right)}{1 + \sum_{k=1}^{n}\left(G_{ik} * \sum_{l=j+1}^{k}\frac{1}{g_l}\right)} \times (V_{in}\alpha_i) \quad (1)$$

where i and j are the row and column indices, G_{ij} is the conductance of the DNA sequence at the $(i,j)^{\text{th}}$grid point, g_l is the interconnect conductance between adjacent memory cells along wordlines, and α_i is a row-specific sneak path parameter (see eqn. (8) in [24]) which is independent of the bias voltage. After the first iteration, the resistance states of DNA memory cells are updated according to the node voltages and the current-voltage relationship. The updated resistance states are used to refine the voltage distribution. This process continues until the voltage difference between two successive iterations

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at each node is within an acceptable tolerance. The voltage distribution obtained after convergence is then used to compute the final read-out current distribution.

For analyzing the performance of the crossbar, we uploaded the 'Lena' image shown in Fig. 3a onto a 128×128 crossbar with an interconnect resistance of 100 KΩ. After simulating the crossbar, the read-out current distribution is obtained, which is shown in Fig. 3b. Finally, the read-out currents are thresholded to obtain the 'reconstructed image' shown in Fig. 3c. A comparison of Figs. 3a and 3c reveal that the reconstructed image has errors, particularly in the north-eastern part. This can be explained by the voltage distribution and the read-out current histogram shown in Figs. 3d and 3e respectively. From Fig. 3d, we observe that the node voltages decrease as we move towards the north-eastern corner of the crossbar. This leads to a reduction in the current difference between the two DNA strands. Consequently, the current distributions for the two DNA strands overlap which is evident in Fig. 3e. This overlap results in an overall bit error rate of 4.52%. The power consumption of the DNA-ROM crossbar can be calculated by summing the product of the node voltage and current overall memory cells. For our simulation setup, the total power consumption was calculated to be 6.75 μW.

V. Conclusion

According to the International Roadmap for Devices and Systems (IRDS 2020), DNA storage technologies are a promising candidate for long-term, large-scale data storage applications. The development of commercially viable DNA-based storage devices is now widely recognized as a critical emergent research area and has rightfully attracted a proliferation of research in recent times. In this paper, we have proposed an electrically readable DNA crossbar storage device with random access capability. The performance of the device has been studied in the context of image storage and retrieval. Although we have considered only two DNA strands as prototypes, the study can be extended to other DNA strands as well.

VI. Acknowledgment

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VII. References

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