# Analogy Between Hydrogen Bonding Network and Microelectronic Circuit

R. P. Rusev, G. V. Angelov, T. B. Takov, M. H. Hristov
Technical University of Sofia, ECAD Laboratory, 8 Kliment Ohridski Str., 1797 Sofia, Bulgaria
rusev@ecad.tu-sofia.bg, gva@ecad.tu-sofia.bg, takov@ecad.tu-sofia.bg, mhristov@ecad.tu-sofia.bg

*Abstract* — **A microelectronic circuit with one input and two outputs that emulates the proton transfer in a hydrogen bonding network is presented. The circuit properties are studied and analyzed using Matlab. Static analysis demonstrates that the circuit can operate as current mirror or amplifier whit different values of the current amplitudes in both outputs. Dynamic analysis shows that the microelectronic circuit can successfully transfer and decode signals.**

*Index Terms* — **Hydrogen bonding network, microelectronic circuits, proton transfer, information processing**

## I. Introduction

Information processing in the near future would require new concepts for solving complex computational problems that are driven by the nanotechnology development and applications. The nature of these problems opens wide range of possibilities for conceiving and applying new ideas and approaches towards finding the optimal solution. One of the most promising approaches is based on methods, algorithms, and structures taken from biological objects. For example, the architecture of human brain and neurons serve as a basis for development of artificial neuron networks for solving complex computational problems [1]. DNA has also proved to be capable of a variety of information processing tasks [2]. A more recent development here is the realization of autonomous molecular automata performing simple logical computations [3]. In [4] a DNA single-electron transistor (SET) is presented as a novel device for single-molecule sequence analysis of DNA strands: the concept is to measure the variations in current through a single electron transistor as a target DNA molecule slithers through a nanocavity integrated between the SET's floating island and gate.

Along with the DNA, proteins are also applicable to solving information processing problems. Bacteriorhodopsin (bR) is one of the proteins investigated for microelectronics applications. It is a convenient model system to study the molecular properties of ion pump that is consisting of hydrogen bonding network. The bR voltage dependence of the photocurrent is compared to the IV-characteristics of conventional microelectronics circuits [5].

In the present paper we present a microelectronic circuit emulating the function of β-lactamase hydrogen bonding network. The hydrogen bonding network (HBN) and its properties are taken from [6]. The I-V characteristics of the conventional microelectronic circuits (I stands for current and V stands for voltage) correspond to K-V characteristics of the HBN (K stands for the proton transfer parameter and V stands for the electrostatic potential), i.e. we derive analogy between the K-V and I-V characteristics of the respective objects since the proton transfer parameter is treated as the electrical current. The signal transfer of the protein HBN is studied by performing dynamic and static analyses.

## II. Equations of the Model

The particular HBN considered in this paper is shown in Fig. 1. Here M182N is assumed to be a current source because it behaves as a donor only. On the other hand D157OD2 behaves as proton acceptor only and can considered as end stage that sums both signals. The other circuit elements are represented as three-terminal networks with equal voltage and different currents in the input and the output terminals.

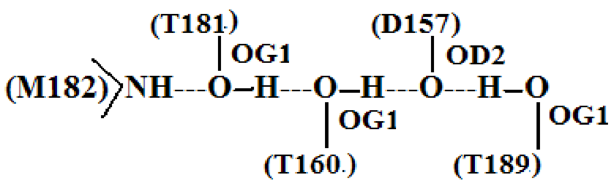


Figure 1. Hydrogen bonding network.(M182) is methionine residue, OG1 is hydroxyl oxygen of threonine residues (T160,181,189), OD2 is carboxyl oxygen of aspartic acid residue (D157)

The corresponding microelectronic circuit emulating the HBN is illustrated in Fig. 2.

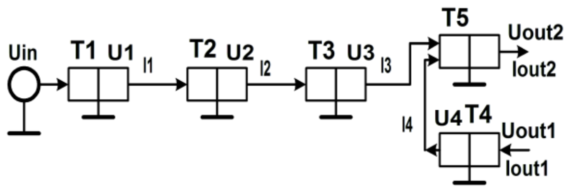


Figure 2. Microelectronic circuit analogous in function to the HBN of Fig. 1.

The currents and voltages of the three- and four-terminal networks and the connections between them are described by polynomials: below are listed the current and voltage equations of block-element T1 of Fig.2 describing the properties of M182N.

$$U_1 = U_{in} \tag{1}$$

$$I_1 = 8*10^{-5}U_1^4 - 7*10^{-5}U_1^3 - 0.001U_1^2 + \\ +0.0048U_1 + 0.2516 \tag{2}$$

Below are listed the current and voltage equations of block-element T2 describing the properties of T181OG1.

$$U_2 = 0.9765U_1 + 0.074 \tag{3}$$

$$I_2 = -0.00011U_2^3 + 0.00032U_2^2 + \\ +0.0012U_2 + 0.0081 \tag{4}$$

Below are listed the current and voltage equations of block-element T3 describing the properties of T160OG1.

$$U_3 = 1.0321U_2 + 0.0519 \tag{5}$$

$$I_3 = 0.00013U_3^3 - 0.0003U_3^2 - \\ - 0.0018U_3 + 0.0104 \tag{6}$$

Below are listed the current and voltage equations of block-element T4 describing the properties of T189OG1 which is the first output of the circuit ($U$1out, $I$1out).

$$U_4 = 0.0031U_1^3 - 0.0616U_1^2 + 1.06U_1 + 0.5256 \tag{7}$$

$$I_4 = +0.76*10^{-5}U_4^3 - 2.1*10^{-5}U_4^2 - \\ - 0.0001U_4 + 0.00066 \tag{8}$$

Below are listed the current and voltage equations of block-element T5 describing the properties of D157OD2 which is the second output of the circuit ($U$2out, $I$2out).

$$U_5 = 0.9608U_4 - 0.0034 \tag{9}$$

$$I_5 = I_3 + I_4 \tag{10}$$

These equations are coded in Matlab [7]. The Matlab code for one of the block-elements is given below (the code for rest elements is similar).

```
U2 = 0.9765*U1 +0.074;
plot(U1,U2);
grid on
title('T2');
xlabel('y text [A]', 'fontsize',12);
ylabel('z text','fontsize',12);
%legend('simulation','data');
set(legend('EKV lc simulation','BSIM3v3
      data',2),'fontsize',12);
pause;
I2 = -0.00011*U2.^3 + 0.00032*U2.^2 + 0.0012*U2 +
      0.0081;
load('fig3_1btl_t181og1.dat');
U2exp = fig3_1btl_t181og1(:,1);
I2exp = fig3_1btl_t181og1(:,2);
plot(U2,I2,U2exp,I2exp,'ro');
grid on
title('T2');
xlabel('U2 [V]', 'fontsize',12);
ylabel('I2','fontsize',12);
% legend('simulation','data');
set(legend('simulation','data',1),'fontsize',12);
pause;
```

## III. ANALYSES

The static and dynamic analyses are done in Matlab.

### A. Static Analysis

First a test to validate how well our model equations predict the hydrogen bonds properties is performed. For all Matlab static simulations we vary $U$in between –2.1 [V] to + 2.65 [V]. Fig. 3 and 4 show that the $I$-$V$ characteristics of the microelectronic circuit input and output elements well emulate the function of the respective biological objects M182N, T189OG1 which properties are investigated in our previous paper [6] (in Fig. 3 and 4 the data from our previous paper are given in red circles). The comparison gives good results for the other elements too which proves that the tested circuit emulates the operation principle of the HBN.

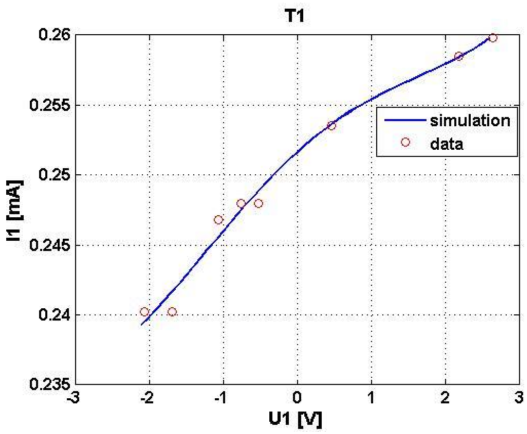


Figure 3. *I-V* characteristic of block-element T1.

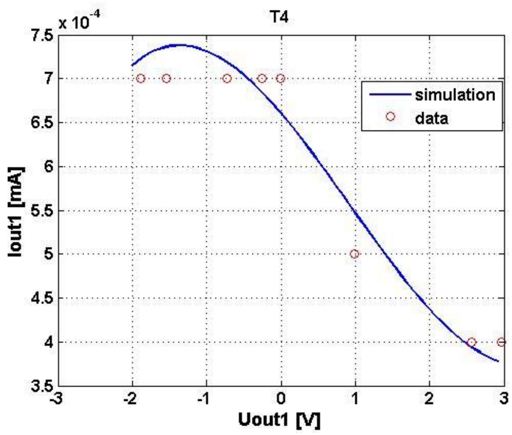


Figure 4. *I-V* characteristic of block-element T4 (the first output of the microelectronic circuit).

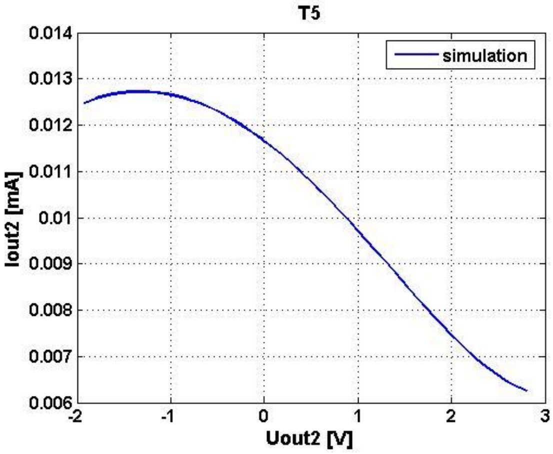


Figure 5. *I-V* characteristic of block-element T4 (the second output of the microelectronic circuit).

The results show that the output voltages are linearly dependent on the input voltage (Fig. 6). While output voltages are nearly equal in magnitude, the difference between the output currents is on the order of three ($I_{out1}$ ~ $10^{-4}$ [mA] and $I_{out2}$ ~ $10^{-1}$ [mA]).

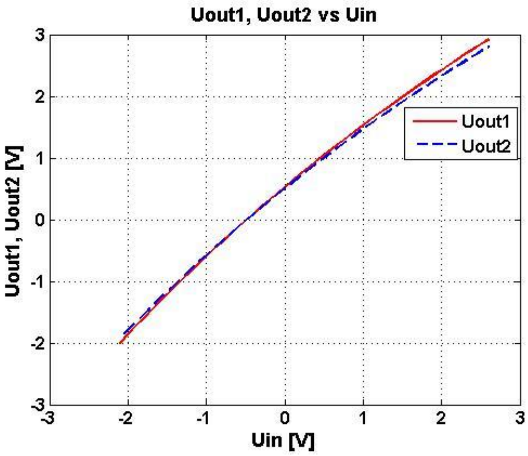


Figure 6. Output voltages at output 1 and output 2 vs. input voltage.

The output characteristics $I_{out1,2} = f(U_{out1,2})$ for the two block-elements are comparable. The curves in Fig. 4 and Fig. 5 can be divided in two regions. In the region between voltages –2 to –0.3 [V] there is no significant change of output currents, hence this circuit could operate as a current mirror. For voltages greater than –0.3 [V] (the second region of operation) the microelectronic circuit behaves as an amplifier.

*B. Dynamic Analysis*

The molecular dynamics of hydrogen bonds is fluctuational in nature which determines the exchange of proton between donors and acceptors and in result donors become acceptors and acceptors — donors. These considerations suggest that the microelectronic circuit can process AC signals. The transconductance of the first output of the microelectronic circuit is $g = \partial I_{out1}/\partial U_{in}$ ~ 0.1 [μA/V] and the transconductance of the second output is $g$ ~ 0.1 [mA/V]. The dynamic resistance of the first output is $R_d = \partial U_{out1}/\partial I_{out1}$=10 MΩ and the dynamic resistance of the second output is $R_d$ ~ 10 kΩ.

It should be noted that the currents in the microelectronic circuit presented here are on the order of mA ($10^{-3}$ A), while the experimental measurements for the currents of the respective HBNs are on the order of pA ($10^{-12}$ A). We have chosen to compare these HBNs to microelectronic circuits where the mA-currents are realistic. That is why the dynamic resistances of the HBNs will be much greater and the trasconductances — much smaller compared to their microelectronic counterparts.

The results of the transient analysis are shown in Fig. 7, 8, 9, 10, 11. The input signal is sinusoidal with amplitude of 2.5 [V] and frequency 100 [GHz].

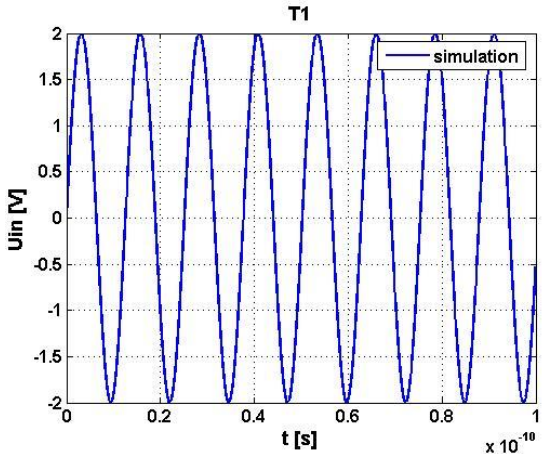


Figure 7. Input voltage vs. time.

As mentioned above the output voltages repeat the input voltage, hence they remain sinusoidal. A typical feature for the two output currents is that they are positive for the negative semi-periods of the input voltage. The currents have different amplitude and are shifted by phase compared to the voltages.

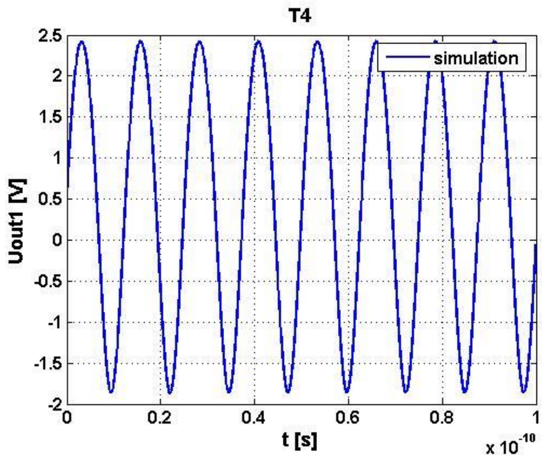


Figure 8. Output voltage at first output vs. time.

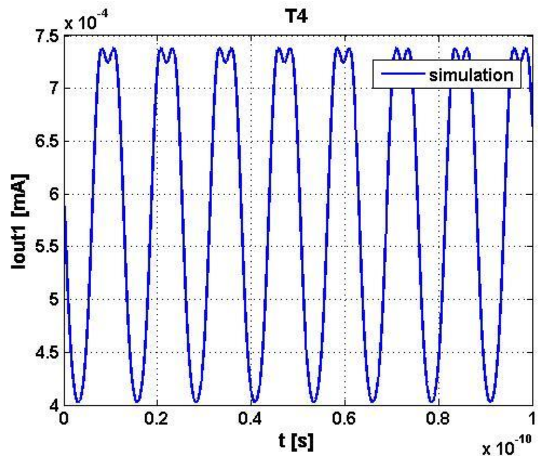


Figure 9. Output current at first output vs. time.

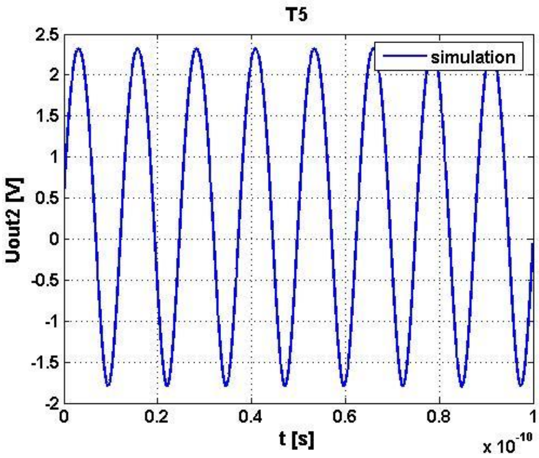


Figure 10. Output voltage at second output vs. time.

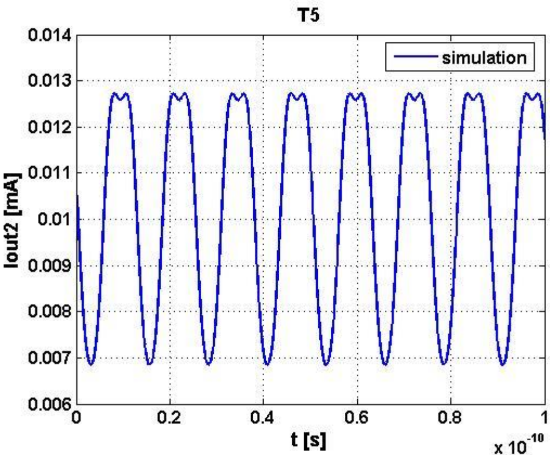


Figure 11. Output current at second output vs. time.

The simulated curves demonstrate that the operation of this circuit is similar to a decoder. Although the discrete elements in the model are ideal (and we cannot perform a frequency analysis) it is well known from the literature that the minimal proton transfer times are on the order of ps ($10^{-12}$ s). So, the considered microelectronic analog of the HBN can process signals with frequencies on the order of hundreds of GHz ($10^{11}$ Hz)

## IV. Conclusion

The proposed microelectronic circuit emulates the function of the hydrogen bonding network. The static analysis shows this circuit can operate as current mirror and amplification with different amplitudes in the outputs. The dynamic analysis demonstrates that the circuit has large dynamic resistance and transfers and processes AC signals. It can be used as decoder with high frequency response.

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## The Authors


Rostislav P. Rusev is a PhD student in the ECAD Laboratory at the Technical University of Sofia. George V. Angelov is assistant professor in Department of Microelectronics, at the TU-Sofia, Tihomir B. Takov is professor in Department of Microelectronics, at the TU-Sofia, and Marin H. Hristov is professor in Department of Microelectronics, TU-Sofia and dean of the Faculty of Electronics Engineering and Technology, TU-Sofia, Bulgaria.


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