Biocircuit for Signal Modulation Based on Hydrogen Bonding Network

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Abstract - **The presented biocircuit emulates proton transfer processes in branching hydrogen bonding network consisting of protein residues and water molecules. The hydrogen bonds equations are coded in Matlab as tree- and four-terminal microelectronic block-elements which are connected in electrical circuit with three outputs. The circuit is further investigated by performing static and dynamic analyses. The static analysis shows that the different circuit's outputs have I-V characteristics similar to tunnel diode and to class B amplifier. The dynamic analysis demonstrates that the biocircuit can serve as signal modulator.**

Keywords – **Proton transfer, hydrogen bonding network, biocircuit, signal modulation, class B amplifier.**

I. Introduction

Proton transport in liquid media and membranes is a fundamental process in living organisms where it is promoted by different proteins like Cytochrome c oxidase (CcO) and/or Bacteriorhodopsin (bR). The CcO operates like nanomachine which converts the electron energy in transmembrane proton electrochemical gradient [1], and the Bacteriorhodopsin (bR) operates like transmembrane proton pump. From microelectronics point of view lots of efforts are made for measuring the proton current by integrating proteins in solid state semiconductor devices [2] using metal-protein-metal junction. On the other hand, several methods for calculation of the proton current in protein hydrogen bonding networks and other systems forming hydrogen bonds such as Benzoic acid crystal [3] and water molecules [4] are developed. In the present paper a microelectronic circuit emulating proton transfer processes in branching hydrogen bonding networks (HBN) is presented. The circuit is investigated by static and dynamic analyses.

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II. Model and Equations

The HBN is taken from [5] and is shown in Figure 1. The branches of the circuit are formed by the Arginine residues R65 and R161, Glutamic acid residue E177 of TEM1 β-lactamase protein. The bonds between the protein residues are formed by water molecules actively participating in the information transfer through the network.

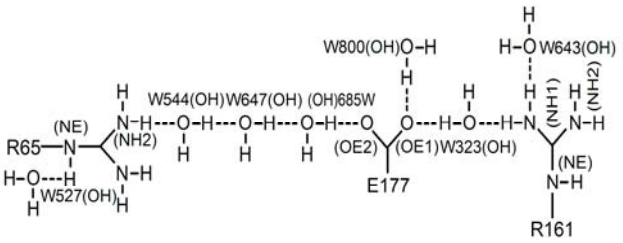

Figure 1. Branching hydrogen bonding network composed of: NH1, NH2, and NE — nitrogen atoms of arginine residues R65 and R161, OE1 and OE2 — carboxyl oxygen atoms of glutamic acid residue E177, OH — are oxygen atoms of water molecules (W323, W544, W527, W643, W647, W685 and W800).

The analogous microelectronic circuit is shown in Fig. 2. Here the hydrogen bonds are interpreted as three- and four-terminal block-elements. The I-V characteristics of the block-elements are proportional to the K-V characteristics of the respective hydrogen bonds investigated in [5]. The current (I) of each block-element represents the proton transfer parameter (K) of each hydrogen bond and the voltage (V) of each block-element represents the electrostatic potential (El. pot.).

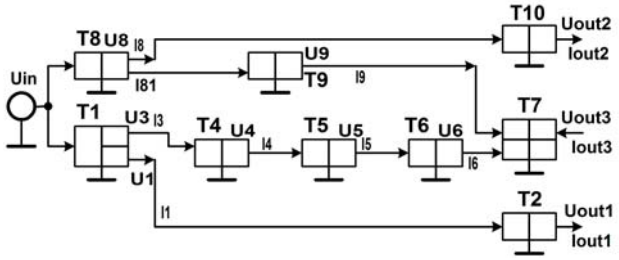

Figure 2. Microelectronic circuit emulating the branching hydrogen bonding network.

The I-V characteristics of the block-elements are described by polynomials of different orders. The polynomials of T1 block-element matching R65 protein residuum are given below. Since R65 is strong proton donor and forms two hydrogen bonds via NH2, and NE atoms its respective matching element T1 has one voltage

controlled input and two different outputs characteristics (U1,I1 and U3,I3):

$$U_1 = [-1.7 : 0.1 : +2.3] \quad (1)$$

$$I_1 = -0.0002*U_1^6 + 0.0017*U_1^5 - 0.0034*U_1^4 - 0.0029*U_1^3 + \\ + 0.0087*U_1^2 + 0.0025*U_1 + 0.3668 \quad (2)$$

$$U_3 = 1.0136*U_1 + 0.0167 \quad (3)$$

$$I_3 = -0.0052*U_3^4 + 0.0132*U_3^3 + 0.0029*U_3^2 - 0.0221*U_3 + \\ + 0.8312 \quad (4)$$

The following protein residue R161 forms two hydrogen bonds only by the NH1 atom. In this reason, it is emulated by T8 with equal voltages at the output and input terminals and different output currents. The respective equations are given below:

$$U_8 = -0.0647*U_1^2 + 1.102U_1 + 1.8304 \quad (5)$$

$$I_8 = -0.0093*U_8^4 + 0.0707*U_8^3 + 0.1762*U_8^2 + 0.1835*U_8 + \\ + 0.7465 \quad (6)$$

$$I_{81} = -0.0005*U_8^3 + 0.0023*U_8^2 - 0.0032*U_8 + 0.0408 \quad (7)$$

The third protein residue building the network is Glutamic acid residue E177 which is strong proton acceptor. It is emulated in the microelectronic circuit by the T7 block-element which output signal (Iout3, Uout3) depends on the current and voltage at the first input terminal (U9, I9) and the voltage of its second input.

$$U_7 = 0.0116*U_9^2 + 0.9413U_9 - 0.2106 \quad (8)$$

$$I_7 = 0.0788*U_7^3 - 0.1039*U_7^2 - 0.3541*U_7 + 2.2594 = I_{out3} \quad (9)$$

The hydrogen bonds formed by water molecules are described with the similar three-terminal block-elements T2, T4, T5, T6, T9, and T10 which equations are shown below:

$$U_2 = 0.9629*U_1 - 0.1139 \quad (10)$$

$$I_2 = I_1 \quad (11)$$

$$U_4 = 0.9465*U_3 - 0.0357 \quad (12)$$

$$I_4 = 6.2*10^{-5}U_4^4 - 0.00036*U_4^3 + 0.0001*U_4^2 + 0.0016*U_4 + \\ + 0.0385 \quad (13)$$

$$U_5 = 0.9683*U_4 - 0.0437 \quad (14)$$

$$I_5 = 0.0021*U_5^4 - 0.0097*U_5^3 + 0.0028*U_5^2 + 0.03*U_5 + \\ + 0.2333 \quad (15)$$

$$U_6 = 0.9411*U_5 - 0.0228 \quad (16)$$

$$I_6 = 0.7072*U_6^3 - 0.5794*U_6^2 - 3.3778*U_6 + 44.728 \quad (17)$$

$$U_{10} = 0.8978*U_8 - 0.9196 \quad (18)$$

$$I_{10} = I_{81} \quad (19)$$

$$U_9 = 0.0329*U_8^2 + 0.8068U_8 - 1.2571 \quad (20)$$

$$I_3 = -0.0052*U_3^4 + 0.0132*U_3^3 + 0.0029*U_3^2 - 0.0221*U_3 + \\ + 2.0351 \quad (21)$$

These polynomials are coded in Matlab [6]. A sample of the code is listed below:

```
% fig5-1bt1
% blok ARG65NE-> 0inp-1out Arguments
 U1 = [-1.7:0.1:2.3];

% function 1 -> 0inp-1out
I1 = -0.0002*U1.^6 + 0.0017*U1.^5 - 0.0034*U1.^4
-0.0029*U1.^3 +0.0087*U1.^2 +0.0025*U1 +0.3668;

load('fig5_1bt1_arg65ne.dat');
U1exp = fig5_1bt1_arg65ne(:,1);
I1exp = fig5_1bt1_arg65ne(:,2);

plot(U1,I1,U1exp,I1exp,'ro');
grid on
title('T1');
xlabel('U1 [V]', 'fontsize',12);
ylabel('I1','fontsize',12);
% legend('simulation','data');
set(legend('simulation','exp data',1),'fontsize',12);
pause;
```

FIGURE 3. PORTION OF MATLAB CODE

III. STATIC ANALYSIS

The static analysis is performed at input voltage between –1.7 and +2.3 [V]. It can be seen from Figure 4 that the three output voltages linearly depend on the input voltage.

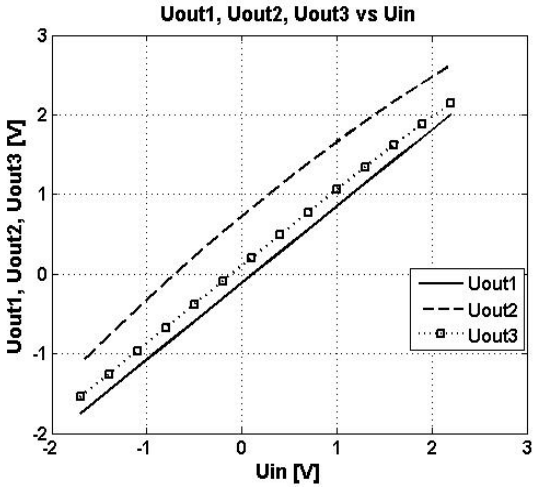

FIGURE 4. OUTPUT VOLTAGES VERSUS INPUT VOLTAGE.

On the other hand the currents in the three output channels of the microelectronic circuit are different functions of the output voltages and of the input voltage. The I-V characteristics of the three output channels are shown in Figures 5, 6, and 7.

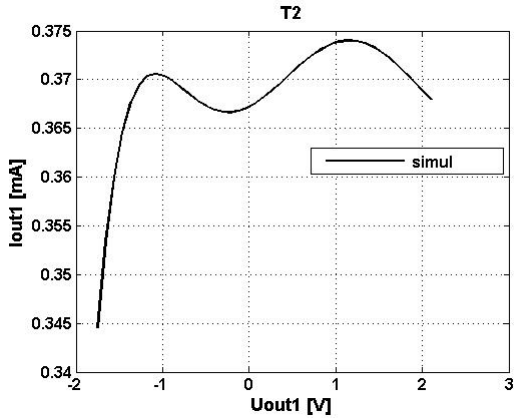

FIGURE 5. I-V CHARACTERISTIC OF THE FIRST CHANNEL OF THE MICROELECTRONIC CIRCUIT.

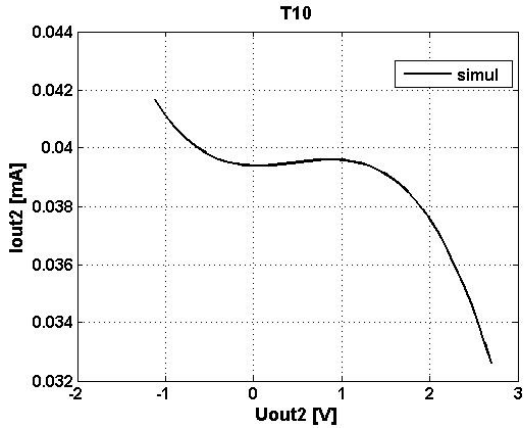

FIGURE 6. I-V CHARACTERISTIC OF THE SECOND CHANNEL OF THE MICROELECTRONIC CIRCUIT.

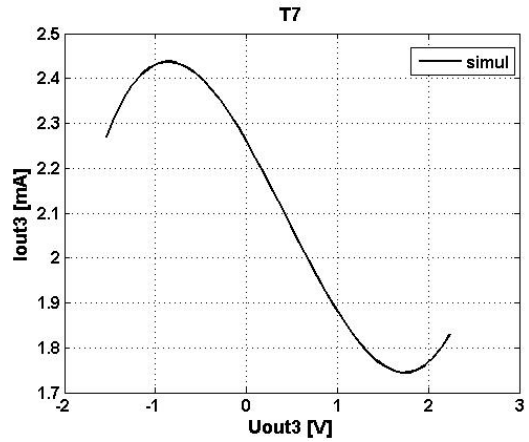

FIGURE 7. I-V CHARACTERISTIC OF THE THIRD CHANNEL OF THE MICROELECTRONIC CIRCUIT (THIS GRAPHICS IS NOT PORTION OF AN PERIODIC FUNCTION).

The currents in the three outputs are positive and they are varying in different intervals. The current in the first output is one order of magnitude lower than the third channel current and the current in the second output is two orders of magnitude lower than the third channel current. From operation point of view this circuit can hardly be compared to a well-known microelectronic circuits and devices. The presented biocircuit is controlled by voltage and the each of its channels has different properties: i) the first channel I-V characteristic is similar to tunnel diode I-V characteristics, ii) the second channel I-V characteristic is similar to shifted output characteristics of class B bipolar amplifier, and iii) the third channel I-V characteristic cannot be compared to a state-of-the-art microelectronic circuit or device.

IV. DYNAMIC ANALYSIS

The dynamic analysis of the circuit is performed by feeding sine input voltage with amplitude between –1.7 and +2.3 [V] at frequency of 100 GHz. The time-dependence of the input voltage is shown in Figure 8.

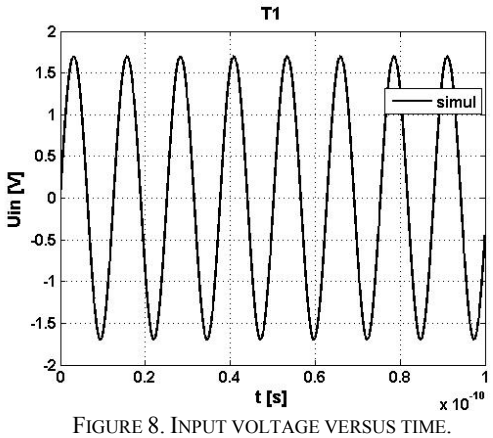

FIGURE 8. INPUT VOLTAGE VERSUS TIME.

In parallel to static analysis, the forms and frequencies of the output voltages are copying the input voltage form and frequency.

Figures 9, 10, and 11 depict the time dependence of the output currents.

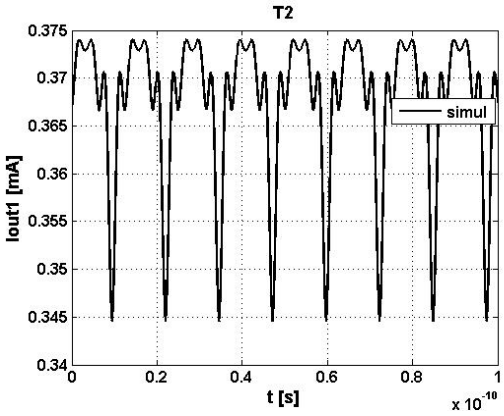

FIGURE 9. FIRST CHANNEL OUTPUT CURRENT VERSUS TIME

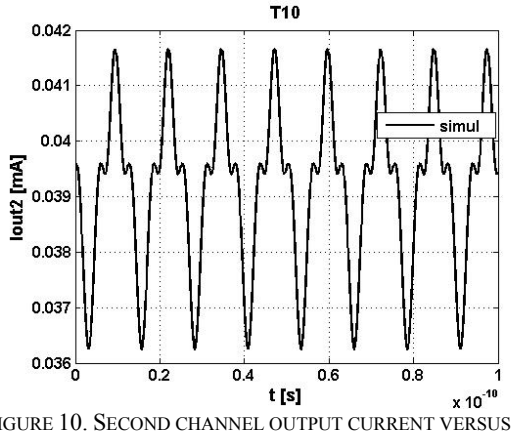

FIGURE 10. SECOND CHANNEL OUTPUT CURRENT VERSUS TIME.

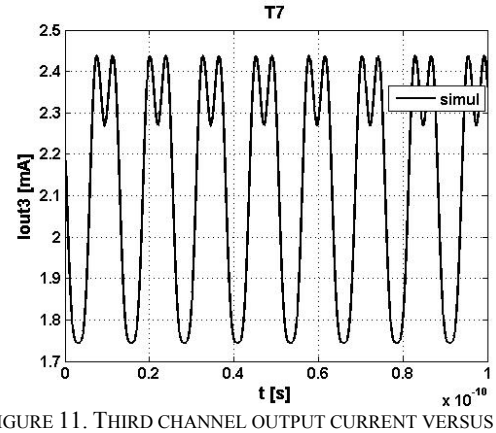

FIGURE 11. THIRD CHANNEL OUTPUT CURRENT VERSUS TIME.

All currents are with positive amplitudes not depending whether the voltage semi-periods are negative or positive. The current in the first channel is in-phase with the input voltage and the currents of the rest of the output channels are anti-phase with the input voltage. Hence, the microelectronic biocircuit can be used for signal modulation.

V. CONCLUSION

The developed microelectronic circuit well emulates the proton transfer processes in branching hydrogen bonding network consisting of protein residues and water molecules. The static analysis shows that each of the three output circuit channels have different I-V characteristics that are similar to the I-V characteristics of tunnel diode and class B amplifier. The dynamic analysis illustrates that the microelectronic circuit can be used for signal modulation.

VI. ACKNOWLEDGMENT

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