DEVELOPMENT AND ANALYSIS OF A SIGNAL TRANSFER CIRCUIT WITH HYDROGEN BONDING

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A microelectronic circuit based on hydrogen bonds is developed and analyzed. The simulations in Matlab demonstrate that the biocircuit object emulates the functionality of conventional electrical circuits. The static analysis shows the circuit is akin to current source while the dynamic analysis demonstrates that the circuit successfully transfers and processes signals (with the option for signal decoding).

Keywords: Hydrogen bonds, microelectronic circuits, bio-computing

1. INTRODUCTION

Information processing requires new concepts for solving the complex problems that are emerging more and more frequently. The difficulties in finding appropriate solutions to these problems are stimulating new analogies and ideas for the application of methods and algorithms taken from the nature. The architecture of brain and natural neuron networks are of big interest for the nanoelectronics. Artificial neuron networks [1] for solving complex computational problems are developed on this basis.

Other unconventional concepts are the biocomputing based on DNA [2]. DNA has a huge potential for information storage – the data density storage is around 10^{21} [bit/cm^3] (i.e. some one trillion of conventional CDs). The main advantage of applying DNA in computing is the possibility for parallel calculations. So far, however, conventional microelectronics cannot enable the right architecture nor the efficient technology for parallel operation.

An interesting relevance taken from the nature is the use of hydrogen bonds as logic gates [3] performing the operations AND, OR, NAND, NOR. Karasev et al. [4] has developed model for topological design of chain biopolymers/polypeptides. The model is based on the property of the polypeptide main chain to for spirals of hydrogen bonds. In this context, the present paper investigates the information transfer via hydrogen bonds for microelectronics applications. The goal is to develop microelectronics circuits that emulate the functional characteristics of a hydrogen bonding network and to study its properties via static and dynamic analyses.

2. MODEL AND EQUATIONS

The hydrogen bonding network and its properties are taken from [5]. The bonding between the elements is shown in Fig. 1; Fig. 2 shows the respective microelectronic circuit that emulates the network in Fig. 1.

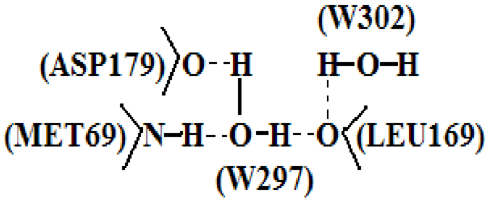

Figure 1. Hydrogen bonding network, where N is nitrogen atom of methionine residue (MET69), O is oxygen atom of water molecules W (297, 302), leucine residue (LEU169) and aspartic acid residue (ASP179).

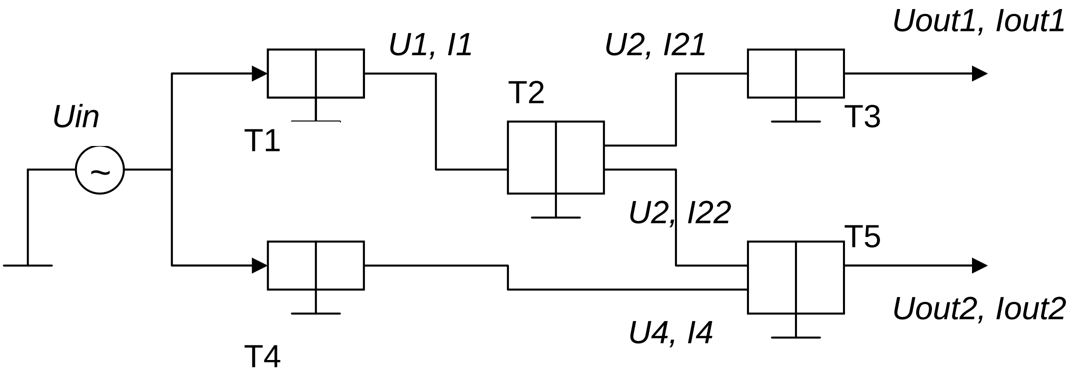

Figure 2. The respective circuit that emulates the function of the network in Fig.1

The heavy atoms, forming the hydrogen bonds, are represented with three- and four-terminal networks. Each three-terminal network has equal input and output voltages and different currents. The equations describing each three-terminal network are

$U_1 = U_{inp}$

$I_1 = -2e-6*U_1.\text{\^{}}6 + 2e-6*U_1.\text{\^{}}5 + 3e-5*U_1.\text{\^{}}4 -6e-5*U_1.\text{\^{}}3 - 1e-6*U_1.\text{\^{}}2 + 4e-5*U_1 + 0.0018$

I_1 and U_1 are the output voltage and current of T1; T1 is a three-terminal network and functionally corresponds to the residue MET69N;

$U_2 = 1.029*U_1 - 0.007;$

$I_{21} = 4e-7*U_2.\text{\^{}}4 +5e-6*U_2.\text{\^{}}3 -1e-5*U_2.\text{\^{}}2 -2e-6*U_2 +0.0002;$

$I_{22} = 0.0001;$

U_2, I_{21}, I_{22} are the voltage and the currents of the two outputs of the four-terminal network T2 that corresponds to W297O. It should be noted that the current does not depend on the voltage.

$U_{out1} = 0.9748*U_2 +0.1928;$

$I_{out1} = 9e-7*U_{out1}.\text{\^{}}4 +4e-6*U_{out1}.\text{\^{}}3 -2e-5*U_{out1}.\text{\^{}}2 +6e-6*U_{out1} +0.0002;$

I_{out1} and U_{out1} are the currents and voltages of the three-terminal network T3 that corresponds to the residue ASP179O. This current and voltage are going to the first output of the overall circuit.

U_4 = 0.0181*U_{inp}.^2 +1.0855*U_{inp} -0.029;
I_4 = -0.0001*U_4.^4 +0.001*U_4.^3 -0.0036*U_4.^2 +0.0043*U_4 +0.4675;

U_4 and I_4 are the voltage and current at the output of the element T4 that corresponds to W302O. This element is going to the second input of the circuit.

U_{out2} = 1.0158*U_4 -0.2319;
I_{out2} = -0.0002*U_{out2}.^4 +0.0008*U_{out2}.^3 -0.0021*U_{out2}.^2 +0.0028*U_{out2} +0.4675 +I22;

U_{out2} and I_{out2} are the voltage and current of the element T5 that functionally corresponds to LEU169O. T5 is a four-terminal network with two inputs, one output, and ground. It sums the two input signals and the output is the second output of the overall circuit.

These equations (not all of them are shown) are implemented in Matlab code [6] to perform the simulations.

3. STATIC ANALYSIS

Having described the circuit and its interconnections in Matlab a static analysis (DC analysis) is carried out. The resulting *IV* characteristics at the outputs are compared to the characteristics obtained in [5]. The characteristics of T1, T3, and T5 are shown in Figures 3, 4, and 5.

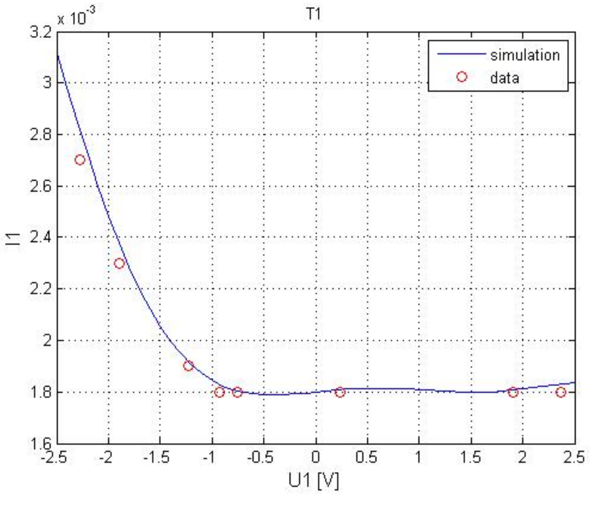

Figure 3. Output characteristic at the output of T1.

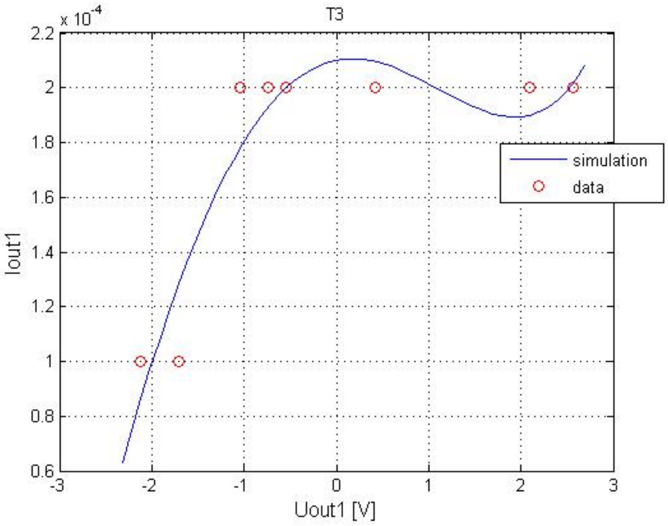

Figure 4. Output characteristic at the output of T3.

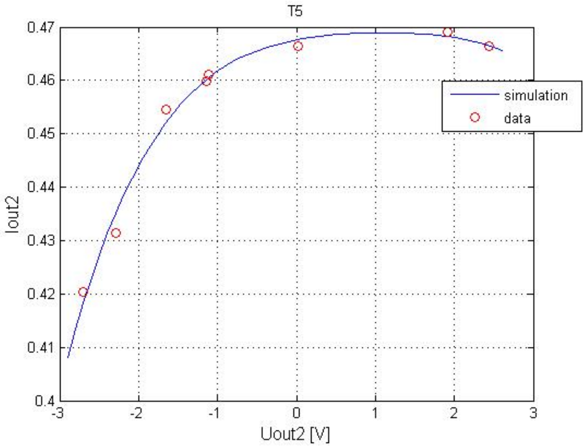

Figure 4. Output characteristic at the output of T5

It can be observed from the figures that the *IV* characteristics equivalent to the microelectronic elements are well reproducing the hydrogen bonds characteristics: Fig. 3 is compared to a diode characteristic, Fig. 5 – to a transistor output characteristic. Fig.4 is analogous to the output characteristic of a tunnel diode; in other studies this characteristic appeared to be similar to the single-electron transistor characteristic which is also based on electron tunneling phenomenon.

The maximum standard deviation in our results (shown with circles in the figures) is 5 %. In other results the error is up to 7 %, i.e. the errors are comparable. Thence, we can conclude that our equations are well reproducing the operation of the bio-object. The simulation tests with the microelectronic circuit are shown in Table 1.

Table 1. Simulation results of the microelectronic circuit in Matlab.

source	Uinp	2.5	1.0000	0	-1	-2.5
out1	Uout1	2.6900	1.1900	0.1850	-0.8200	-2.3220
out1	Iout1	1.9670E-04	1.8750E-04	2.0000E-04	1.8000E-04	5.4000E-05
out2	Uout2	2.5600	0.9000	-0.2100	-1.3200	-2.9800
out2	Iout2	0.4656	0.4689	0.4671	0.4572	0.4080

The supply voltage is in the range of –2.5 to +2.5 V. It is obtained for media with pH between 0 to 14 units. For other values of the voltage (out of this range) a denaturalization of the protein might occur and accordingly, the corresponding electrical circuit would fail. On the other hand, the output voltages repeat the input voltage and the current in the outputs is varying in an extremely narrow interval. Hence, this circuit might emulate a current source.

4. DYNAMIC ANALYSIS

According to the micro-reciprocity principle after proton transfer donors become acceptors and acceptors — donors. Due to molecular dynamics this process has fluctuations and implies oscillations in proton transfer systems. This is effect is studied here by enabling the circuit to process alternating signals. For this reason a sinusoidal signal is fed to the input of the microelectronic circuit. Figures 6, 7, 8, 9, and 10 show the time dependence of the input voltage, the output voltages and the currents at the first and second outputs.

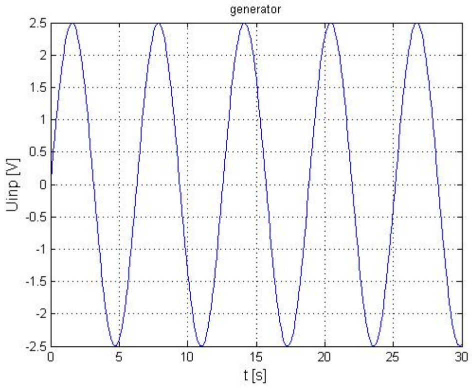

Figure 6. Uin vs. time.

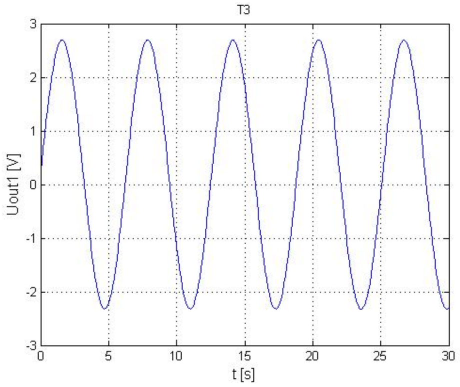

Figure 7. Uout1 vs. time.

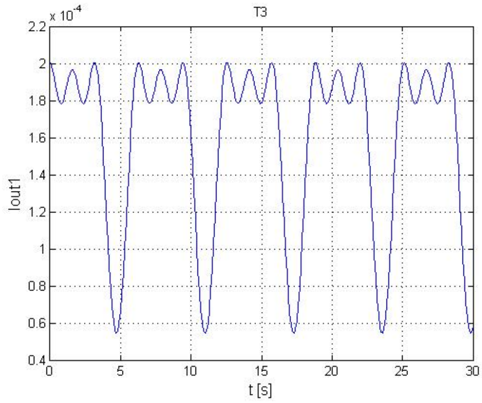

Figure 8. Iout1 vs. time.

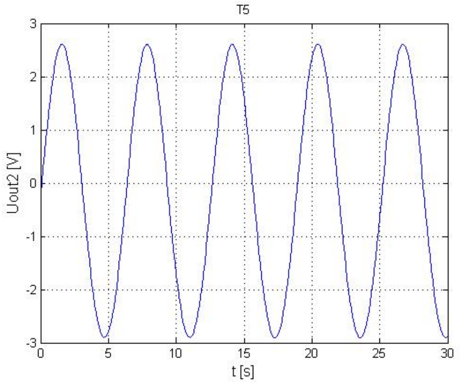

Figure 9. Uout2 vs. time.

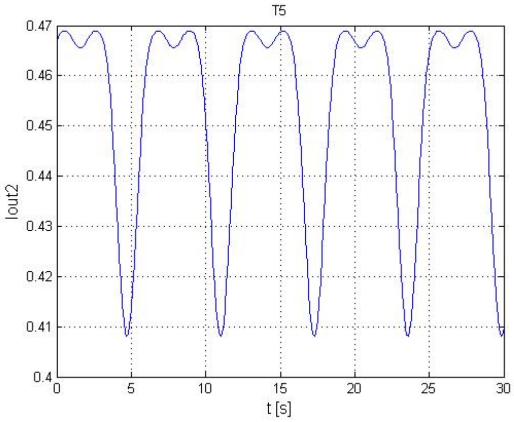

Figure 10. Iout2 vs. time.

It can be seen in the figures that the output voltages repeat the form of the input voltage but differ in amplitude. During the negative semi-periods of the input voltage the two currents are positive. Therefore, this circuit might emulate a decoder. Such circuits should be small-sized (approx. 1 nm) and high speed. In the simulations we are using ideal elements, so we cannot perform frequency analysis but from the literature it is known that the minimal times for proton transfer are on the order of

10^{-12} s [7]. Therefore, the present circuit should process signals with frequency of 10^{12} Hz.

5. CONCLUSION

The developed microelectronic circuit emulates the function of the hydrogen bonds network. The static analysis shows that it can be used as a current source. The dynamic analysis proves that the circuit can successfully transfer and process alternating signals and might be used as a decoder with extremely small size and high speed of operation.

6. ACKNOWLEDGEMENT

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7. REFERENCES

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