Work Book of NATO ARW, Frontiers in molecular-scale science and technology of nanocarbon, nanosilicon and biopolymer integrated nanosystems, Ilmenau – 2003. 10. Ivanyuta O., Tsamis C., Scharff P. et al, DNA, DNA/metal nanoparticles, DNA/nanocarbon and macrocyclic metal complex/fullerene molecular building blocks for nanosystems: electronics and sensing //In Book Frontiers of multifunctional integrated nanosystems, Ed. by Buzaneva E, Scharff P., NATO Science Series II, Mathematics, Physics and Chemistry – NAII. Dordrecht. – 2004. – Vol 152. – P. 251–276. 11. Andersen ES, Dong M, Nielsen M., Self-assembly of a nanoscale DNA box with a controllable lid. // Nature – 2009 – Vol. 459 – P. 7243. 12. Aldaye FA, Palmer AL, Sleiman H.,F Assembling materials with DNA as the guide. // Science. – 2008. –Vol 321, – P. 5897. 13. Bogdan D., Morari C., Electronic Properties of DNA Nucleosides Adsorbed on a Au(100) Surface. // J. Phys. Chem. C. – 2012. – Vol. 116 (13). – P. 7351–7359. 14. Calborean A., Buimaga-Larinca L., DFT simulation of vibrational properties of adenine adsorbed on gold surface: The effect of periodic boundary conditions // Computational and Theoretical Chemistry. – 2012. – Vol. 993. – P. 106–112. 15. Hughes-Stamm S.R., Ashton K.J., Daal A., Assessment of DNA degradation and the genotyping success of highly degraded samples. // Int. J. Legal Med. – 2011. – Vol. 125(3). – P. 341–348. 16. Isaksson J., Acharya S, Barman J, et.al., Single-stranded adenine-rich DNA and RNA retain structural characteristics of their respective double-stranded conformations and show directional differences in stacking pattern. // Biochemistry. – 2004. – Vol. 43(51). – P. 15996–6010. 17. Ivanyuta A.N., Prokopenko O.V. Sensing of DNA polymerised molecules in networks // In Proceedings of PLMMP-2010 5th International Conference Physics of Liquid Matter: Modern Problems. – 2010. 18. Ivanyuta O., Gobsh G., Scharff P. et al., Photonics of mimetic biomolecules: the photoluminescence spectroscopy of cysteine molecules in thin layer // In Proceedings of the VI International Conference on Electronics and Applied Physics. – 2010. 19. Rosa M., Corni S, Di Felice R., A Density Functional Theory Study of Cytosine on Au(111) // J. Physical Chemistry. – 2012 . – Vol. 116(40). – P. 21366–21373. 20. Sun W., Di Felice R., Nature of the Interaction between Natural and Size-Expanded Guanine with Gold Clusters: A Density Functional Theory Study. // J. Physical Chemistry. – 2012. – Vol. 116(40). – in print. 21. Watanabe H., Manabe C., Shigematsu T et al., Single molecule DNA device measured with triple-probe atomic force microscope // Appl. Phys. Lett. – 2001. – Vol 79. – P. 2462–2465.

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ЕЛЕКТРОФІЗИЧНІ ВЛАСТИВОСТІ *ДНК* І *ДНК*: *AU* МОЛЕКУЛЯРНИХ КЛАСТЕРІВ НА САПФІРІ

Покриття ДНК, ДНК: Au, як кластери з гелієвих розчинів можуть виявляти магнітну й електричну активність у біосенсорній системі та виявити функціональні властивості для мікрохвильової техніки. Дослідження було зосереджено на аналізі їх ВАХ та спектрів методами розпізнавання і прогнозування цих молекулярних взаємодій на основі їх первинної структури та взаємозв'язку з фізико-хімічними властивостями. Результати показали, що ці молекулярні шари кластерів на підкладках Al_2O_3 можуть проводити електричний струм і реагувати на потужність НВЧ.

Ключові слова: ДНК, UV-VIS-NIR спектри, точкове джерело низько енергетичних електронів, вольт-амперна характеристика.

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ЭЛЕКТРОФИЗИЧЕСКИЕ СВОЙСТВА *ДНК* И *ДНК*: *AU* МОЛЕКУЛЯРНЫХ КЛАСТЕРОВ НА САПФИРЕ.

Покрытие ДНК , ДНК:Au, как кластеры с гелиевых растворов могут проявлять магнитную и электрическую активность в биосенсорной системе и функциональные свойства для микроволновой техники. Исследование было сосредоточено на анализе их ВАХ и спектров методами распознавания и прогнозирования этих взаимодействий на основе их первичной структуры и взаимосвязи с физико - химическими свойствами. Результаты показали, что эти молекулярные слои кластеров на подложке Al_2O_3 могут проводить электрический ток и реагировать на мощность СВЧ.

Ключевые слова: ДНК, UV-VIS-NIR спектры, точечный источник низко энергетических электронов, вольт-амперная характеристика.

UDC 577.3

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INFLUENCE OF RECOVERY MODEL PARAMETERS ON SYNCHRONIZATION IN NEURAL CORTICAL STRUCTURE DURING DESCENDING INFORMATION TRANSFER

Neurons interaction in networks with complex dynamics was investigated, the synchronization phenomenon for descending information process in cortical column was considered. The synchronization coefficient dependency on different variations of Izhikevich model parameters is depicted on corresponding plots. Visual study of network synchronization is performed by means of raster plots. Synchronization coefficients on different layers of cortical column were compared. Proved that time-scale parameter of membrane potential recovery variable has the weakest influence on network synchronization.

Keywords: synchronization coefficient, Izhikevich model, cortical network, descending information process.

Problem statement. Last years studies of brain neuron networks and principles of information presentation and transformation in the brain are of great interest. Today number of tools and resources for neurophysiological experiments allows us to get more information about functioning of different brain neuron networks. One of the main directions in this science brunch is development of physical and mathematical neuron models that describe basic functional possibilities of neurons and convenient for theoretical researches. Such models are very popular in neurons researching to solve one of the main neurophysiological and biophysical problems: determination how information flows in the network is related to network's topology.

Analysis of recent researches and publications. Active researches of brain's structural organization summarized that the main principle of brain's organizing is the modularized structure and partial information processing. [8] Neocortex is responsible for thinking, speaking and other processes of nervous system and has the most representative modularized organization. Aggregation of cells and links in the cortex into horizontal layers may lead to the conclusion that main interactions in the brain take place in the horizontal planes. But in the 1930-s Spanish scientist Rafael Lorente de No [7, 6] first supposed that cortical processes are local and take place in the vertical columns. Lorente de No assumed that neurons in such structures are associated into closed networks with ring topology. It must be mentioned that till nowadays scientists have no consensus about cortical column's form (cylinder, cone, line, ensemble, "barrel" and others) [9, 10]. Nevertheless comparison of results from different functional researches shows the existence of vertical neuron groups. Hebb [4] hypothesized that neurons ensemble is organized as 3d network consisted of elements with different functional states. Synaptic currents in such network amplify each other by synchronous occurrences. Since the beginning of 60 years this point of view gets demonstrative confirmation. In 1957 Mountcasle noticed that somato-sensory cat's cortex is organized into "elementary functional units" – vertically oriented cell columns. Any column has 110 neurons [8], and this number doesn't dependent on the species e.g. cat, rat, human etc. Columns are considered as the neocortex's evolutionary unit and there are many thoughts about their structural and functional transformations.

Exact structure of the neuron cortex module and coupling parameters are unknown. Analysis of network dynamics [2] can be held for different column structures and topologies. Simulation results can be compared with neurophysiological experiments data to obtain additional knowledge about network topology. Now dynamical research is devoted to neurons synchronization [8]. Synchronization is a central mechanism of neural informational processes that connects different parts of brain. Experimental results show that the synchronous neuron's activity is responsible for visual recognition of whole subject and for information transformation. On the other side the synchronization presence is a reason of pathology and plays an important role in such neural diseases as epilepsy.

Paper goal. This work is devoted to synchronization researching in Izhikevich's neuron network, especially to dependency of synchronization coefficient on variation of neural states in cortical column.

Materials and methods. We considered neural networks consisted of 110 neural elements with different regimes: regular spikes, chaotic spikes, regular and chaotic bursting, etc. All investigated structures are six-layer homogeneous networks similar to cortical columns. Microscopic observations prove that density and form of cells vary from the top to the deep in the cortex. Such differences correspond to horizontal layers. The upper layer, which is called the first, has little cells and consists mainly of axons. In our work there are 9 neurons at the first layer. The second and the third layers are the similar, and each of them has 11 neurons. The fourth layer has 15 neurons, the fifth – 17. The sixth layer is the deepest and strongly differs from others; it has a big amount of neurons, in our case it consists of 47 neurons. (*fig. 1*). Each neuron is connected with each neuron from its own layer and from the next layer. Layers in column are connected by axons and synapses.

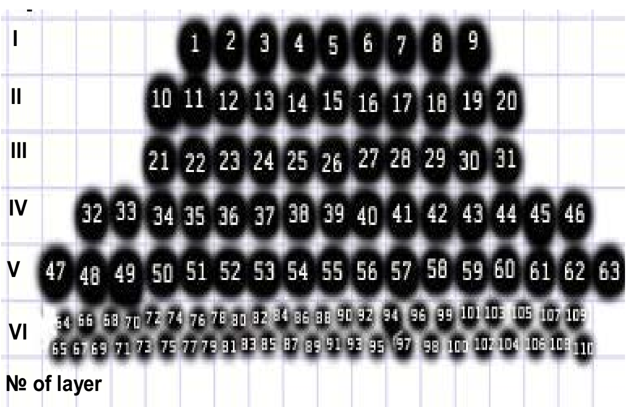

Fig. 1. The hierarchical structure of investigated cortical column

A very interesting question arises: how such little cortical parts may send and get information from the top to the deep in the cortex and what is happen with neural dynamics in such case?

We are interested in the dependence of the synchronization phenomenon on different variation of Izhikevich model parameters. [5]. It is two-compartment model that contains an additional requirement for cell membrane discharge:

$$\frac{dv}{dt} = 0.04v^2 + 5v + 140 - u + I\,,\ \ \frac{du}{dt} = a(bv - u),$$

$$v \leftarrow c, u \leftarrow u + d\ ,\ \textit{if } v>=30\ mV,$$

where v and u are the dimensionless membrane potential and membrane potential recovery variables respectively; *a, b, c* and *d* – dimensionless parameters. The variable u simulates the activation of ionic K^+ currents and the deactivation of ionic Na^+ currents and provides negative feedback to v. Variable I simulates external currents.

Various choices of the parameters result in various intrinsic firing patterns, including those exhibited by the known types of neocortical and thalamic neurons [3]. So in this work we investigated the dependence of synchronization coefficient from variation of neural regimes in cortical column.

Results and discussions. We considered the descending information flow in neural structure. Information goes from the top to deep in the cortical column and hasn't a direct way (*fig. 2)*. Descending connections start at the sixth layer cells and reaches the first layer of the lower cortical regions. The axon spreads to large distances in the first layer. This layer has very few cells. Cells in the second and fifth layers have dendrite couplings with the first layer. Thus cells may be excited by reverse connections that go from the first layer. Axons from the second and the third layers provide synaptic currents to the fifth layer. Thus we can say that the information path from the top to the deep is complex. Information may be divided into different directions. This distribution occurs in the first layer. The reverse information flow coupling begins from the cells of the sixth layer in upper hierarchical region, and then it comes to the first layer of the lower cortical regions. Some cells of the second, third and fifth layers in the lower hierarchical regions are excited. Thus cells of the sixth layer are also excited and then the information goes to lower and lower hierarchical columns.

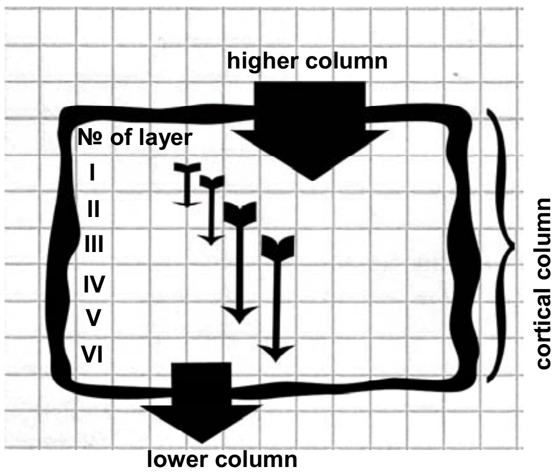

Fig. 2. The descending information flow

As we know from [5] – the parameter *a* describes the time scale of the recovery variable *u*. Smaller values result in slower recovery. A typical value is *a=0.02*. For the descending information flow dependence of synchronization coefficient changes on changes of parameter *a* for the whole cortical column (*fig. 3*) and for each layer separately (*fig. 4*) was investigated.

From *fig. 3* we can see that for descending information flow the maximum value of synchronization coefficient equals *k=0.27* is reached at *a=0.03*. From *fig. 4* we can see that on the first layer of the structure the synchronization coefficient is bigger than on other layers of cortical structure for all values of parameter *a.* The reason of this phenomenon is that the first layer is the input layer that gets an applied synaptic current which flows from upper cortical regions. For parameter value *a=0.03* the raster plot for descending information flow in the cortical column (*fig. 5*) was constructed. Neural dynamics looks like *intrinsically bursting (fig. 6)*.

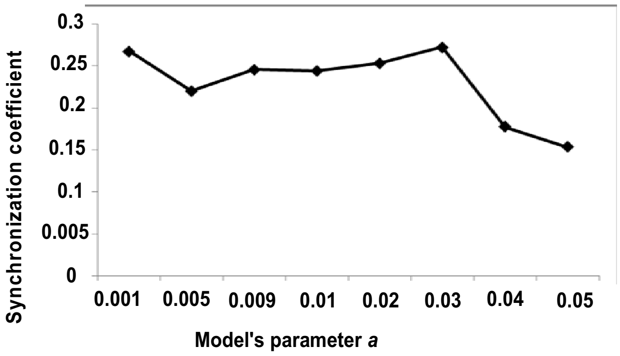

Fig. 3. Dependence of synchronization coefficient on parameter a

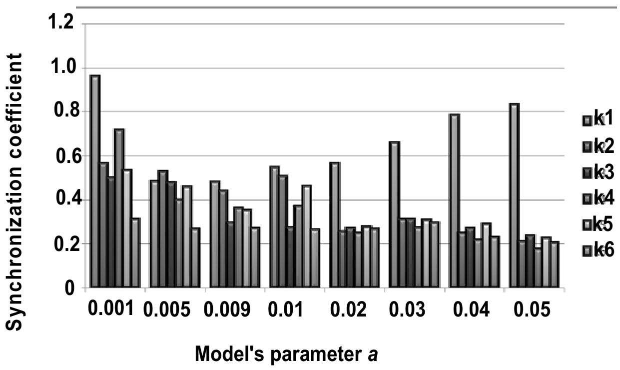

Fig. 4. Layer dependence of synchronization coefficient on parameter a

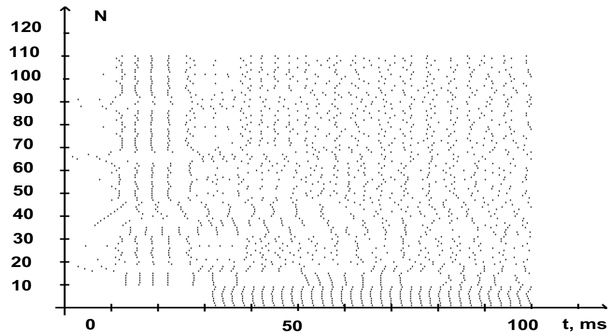

Fig. 5. The raster plot for a=0.03

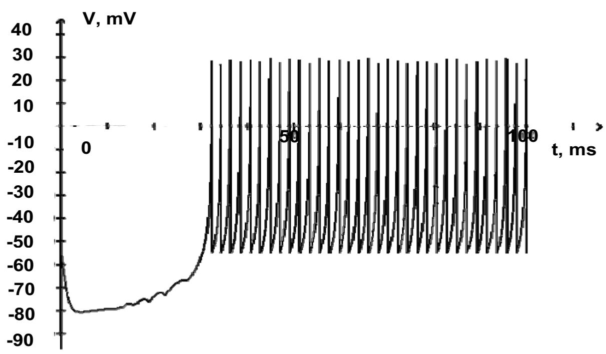

Fig. 6. Neural dynamics for a=0.03

Then the synchronization coefficient changes dependent on changes of parameter *b* for the whole cortical column (*fig. 7)* was investigated. The diagram of synchronization coefficient dependence on parameter *b* was constructed (*fig. 8*) for different layers. From [5] the parameter *b* describes the sensitivity of the recovery variable *u* to the subthreshold fluctuations of the membrane potential *v*. The large values of *v* and *u* lead to the large possible subthreshold oscillations and low-threshold spiking dynamics. A typical value is *b=0.2.*

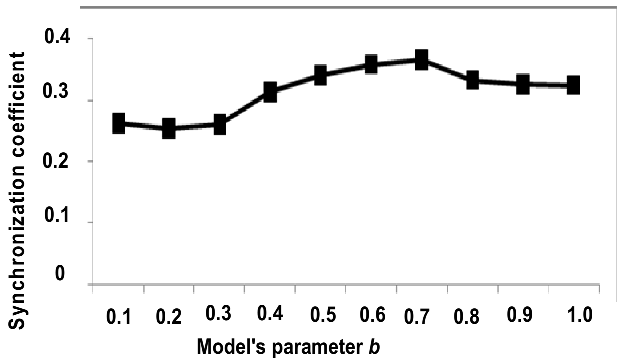

Fig. 7. Dependence of synchronization coefficient on parameter b

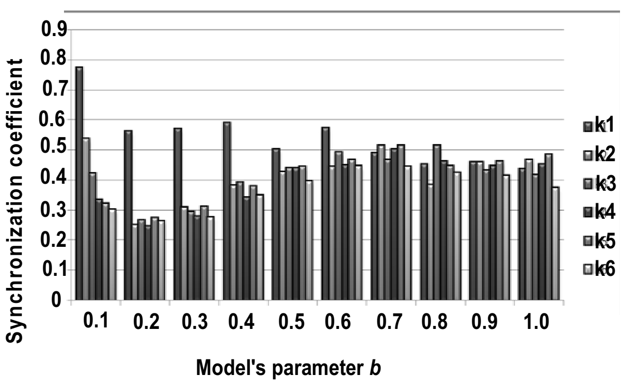

Fig. 8. Layer dependence of synchronization coefficient on parameter b

From *fig. 7* we can see that the synchronization coefficient changes very fluently (~10%) while parameter *b* varying. The maximum value of the synchronization coefficient equals *k=0.365* is achieved at *b=0.7.* From the diagram *(fig. 8),* we can see that the the first input layer has significantly different dynamics of synchronization coefficient changes compared to other layers. For *b=0.7* the raster plot for descending information flow in the cortical column (*fig. 9*) was constructed. Neural dynamics looks like *intrinsically bursting (fig. 10)*.

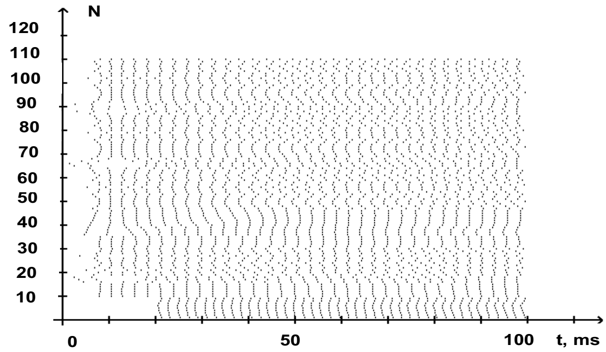

Fig. 9. The raster plot for b=0.7

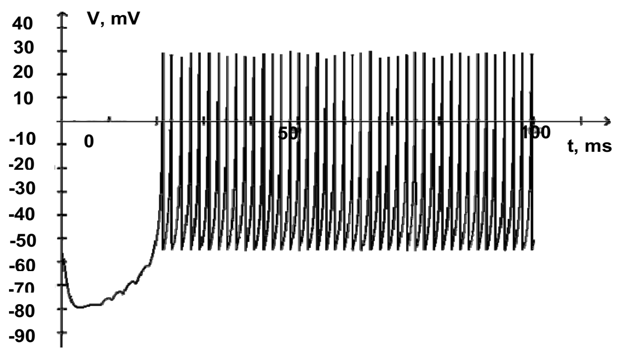

Fig. 10. Neural dynamics for b=0.7

Conclusions. Neurons activity in the cortical column model is changed from bursting to spiking activities when considering from the first to the sixth layer. Researches of synchronization coefficient dependency from changing Izhykevich model' parameters showed:

- presence of parameters, for which the complex neural network dynamics is possible;
- the synchronization coefficient reaches its maximum at:
  - for a=0.03 → k=0.27;
  - for b=0.7 → k=0.365;
- cortical column is less synchronized during changing of parameter a: the synchronization coefficient k – 25−30%;

We can conclude that the time-scale parameter of the membrane potential recovery variable has the weakest influence on synchronization in neocortex. Smaller values result in slower recovery. To enhance synchronization activity in neurons mention above the sensitivity of the recovery variable to the subthreshold fluctuations of the membrane potential should be increased. This fact may be useful for influence on epileptic activity.

Reference

1.Abarbanel G. D., Rabinovich M. I.,Selverston A. Sinhronizacija v nejronnyh ansambljah // Uspehi fizicheskih nauk, Tom 166, №4, – 1996. – s. 363–390. 2. Borisjuk G. N., Borisjuk R. M., Kazanovich Ja. B., Ivannickij G. R.Modeli dinamiki nejronnoj aktivnosti pri obrabotke informacii mozgom – itogi "desjatiletija" // Uspehi fizicheskih nauk, tom 172, №10, 2002. – s. 1189–1214. 3. Izhikevich E. M. Simple model of spiking neurons // IEEE Transactions on Neural Networks. – 2003. – 14, №6. – P. 1569–1572. 4. Hebb D.O. The organization of behaviour. A neurophysiological theory. New York 1949. 335p. 5. Kochubej S. A.. Osobennostu rascheta koefficienta sinhronizacii nejronnyh setej // Visnyk Dnipropetrovskogo universytetu. Biologija. Ekologija. – 2009. – Vyp. 17, t. 2. – s. 55–62. 6. Lorento de No R. Analysis of the activity of the chains of internuncial neurons // J.Neurophysiol. 1939. V.1. P. 208–217. 7. Lorento de No R. Studies of structure of the cerebral cortex // J.Psychol. Neurol. 1933.V. 45. P. 381–392. 8. Mauntkasl V., Organizujuschij princip funkcii mozga: elementarnyj modul i raspredelennaja sistema // Edelman Dz., Mauntkasl V. Razumnyj mozg. – M.: Mir, 1981. 9. Serkov F. N. Elektrofiziologija vysshyh otdelov sluhovoj sistemy. – Kiev: Nauk. dumka. – 1977. – 215s. 10. Towe A.Z. Notes on the hypothesis of columnar organization in somato-sensory cerebral cortex. //Brain. Behav. and Evolut. 1975. V. 11. N 1. P.16–47.

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ВПЛИВ ВІДНОВЛЮЮЧИХ ПАРАМЕТРІВ МОДЕЛІ НА МЕРЕЖЕВІ СИНХРОНІЗАЦІЙНІ ХАРАКТЕРИСТИКИ НИЗХІДНОГО ІНФОРМАЦІЙНОГО ПРОЦЕСУ В НЕЙРОННІЙ КОРТИКАЛЬНІЙ СТРУКТУРІ

У роботі досліджено характер взаємодії нейронів у мережах зі складною динамікою, розглянуто явище синхронізації для низхідного інформаційного процесу у кортикальній колонці. Залежність коефіцієнтів синхронізації від варіювання різних параметрів моделі нейрона Іжикевича відображено на відповідних графіках. Для візуальної оцінки синхронізації побудовано растри спайкової активності. Побудовано діаграми для порівняння коефіцієнтів синхронізації на кожному з шарів кортикальної колонки. Показано, що на синхронізацію найменший вплив має зміна часового параметру відновлення мембранного потенціалу.

Ключові слова: коефіцієнт синхронізації, модель Іжикевича, кортикальна нейромережа, низхідний інформаційний потік.

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ВЛИЯНИЕ ВОССТАНОВИТЕЛЬНЫХ ПАРАМЕТРОВ МОДЕЛИ НА СЕТЕВЫЕ СИНХРОНИЗАЦИОННЫЕ ХАРАКТЕРИСТИКИ НИСХОДЯЩЕГО ИНФОРМАЦИОННОГО ПРОЦЕССА В НЕЙРОННОЙ КОРТИКАЛЬНОЙ СТРУКТУРЕ

В работе исследован характер взаимодействия нейронов в сетях со сложной динамикой, рассмотрено явление синхронизации для нисходящего информационного процесса в кортикальной колонке. Зависимость коэффициентов синхронизации от варьирования различных параметров модели нейрона Ижикевича показана на соответствующих графиках. Для визуальной оценки синхронизации построены растры спайковой активности. Построены диаграммы для сравнения коэффициентов синхронизации на каждом из слоев кортикальной колонки. Показано, что на синхронизацию наименьшее влияние имеет переменная временного параметра восстановления мембранного потенциала.

Ключевые слова: коэффициент синхронизации, модель Ижикевича, кортикальная нейросеть, нисходящий информационный поток.

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COMBUSTION REACTOR SIMULATION USING CELLULAR AUTOMATONS

Evolution process in a system of burning fuel in a limited reactor with high-level substance mixing is analyzed. Demonstrated that the system tends toward decreasing total combustion front length and suppressing smaller dissipative structures by bigger ones. It is shown that little temperature noise affects those structures similar to high diffusion. Also the relation between coefficients used in theoretical model and stationary cluster formation is derived.

Key words: burning process, feedback, equilibrium state, dissipative structures, cellular automatons.

Introduction. Ordinary models describing the burning process of a combustion agent use dynamic coordinate-dependent fuel distribution. Such systems are developed for solid or fluid fuels [1, 2] and assume using the inhibitor method to achieve correct results [6].

Another option determining our current interest consists in systems with high-level substance mixing where strong feedback based on general fuel concentration is present.

The examples are high-movable gas jet burning and glow discharge between two flat electrodes. Points of interest in such system are conditions for occurrences of one or another state and their time and parameters variation stability.

In this paper we demonstrate typical solutions obtained by rarely used cellular automatons method [4] and explain why such method was chosen to solve the theoretical