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FUTURE OF NANO MATERIALS WORLD IS A CREATION OF KNOWLEDGE BASE

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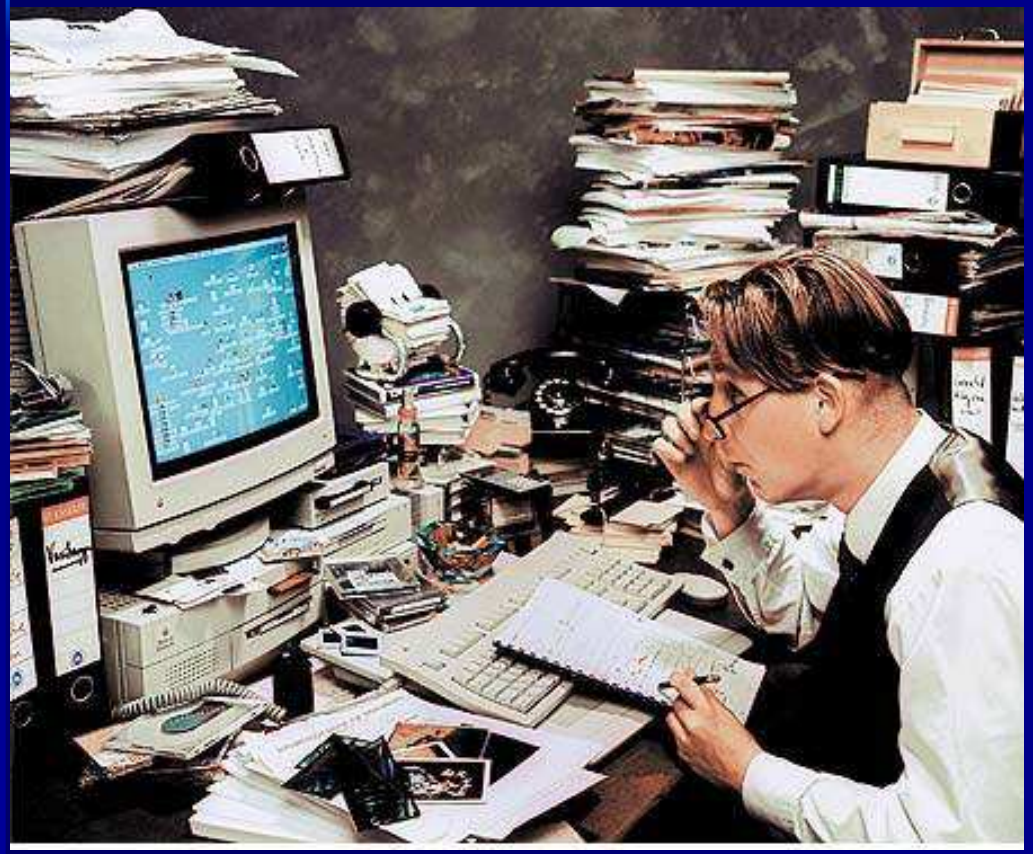
Before



When you work upon
a problem solution,
always useful

to know answers!

What does an experiment means?

- An experiment means that you have tables and graphics.
- The question is how we can increase the significance of the experimental data? Yow we can we see beyond the experimental data? How we can do this?
- A lot of experimental data obtained in the world!
- How we can summarize them? Can we imagine them in a computational model, which absorbs all the tables of experimental data obtained in the world of nanomaterials, and present them in the form of all possible graphics?
- Will this computational model to solve the direct and inverse problem ?
- Will this computational model to predict the results of the experiments have not yet?

Data Mining Approach of Data Analysis

- The Data Mining is a complex of contemporary tools for data analyzing and modeling
- The Data Mining involves such kinds of tools as artificial neural networks (ANN), self-organization maps, decision trees, etc.
- ANN have a head role from the point of view of creation of a calculation models. Other tools of Data Mining have the auxiliary role for data choosing for creation of ANN calculation models.

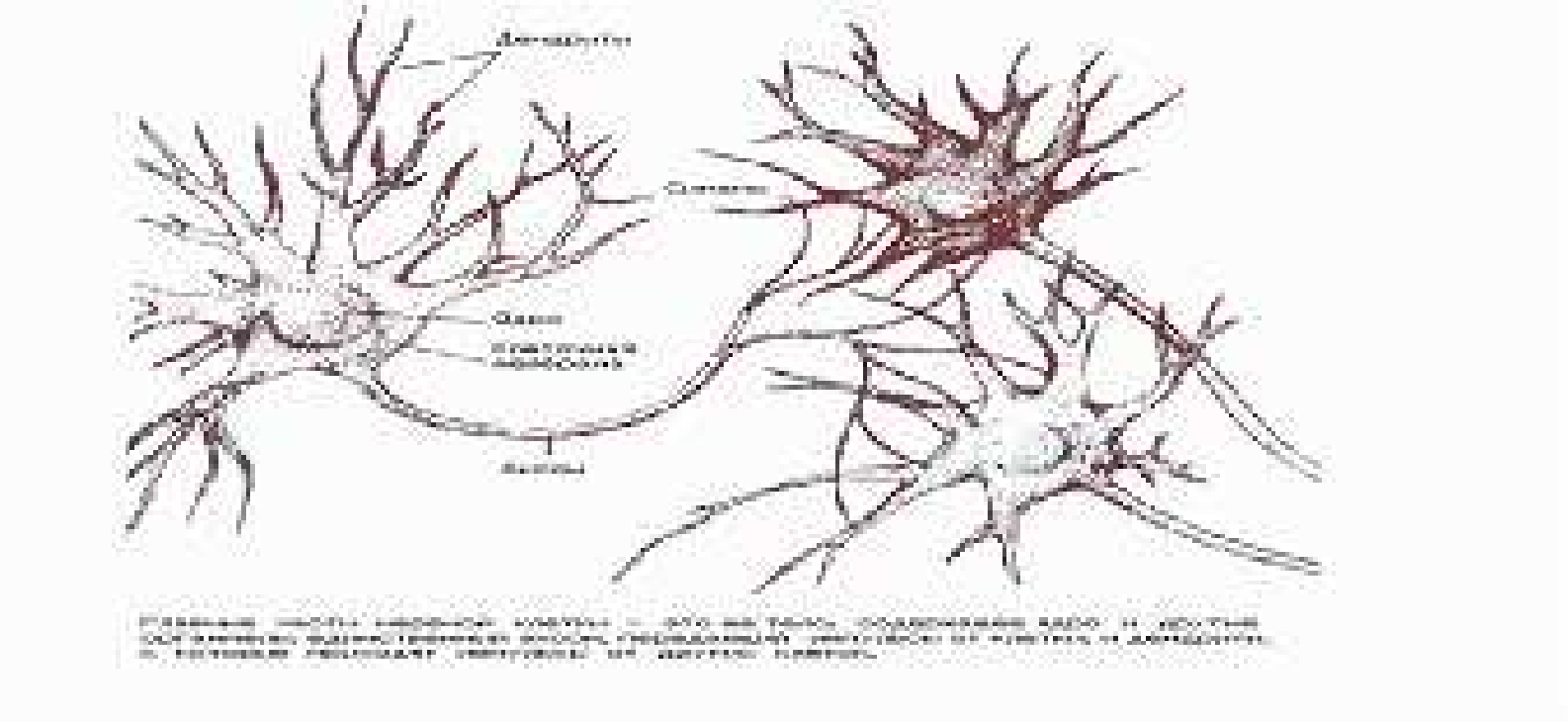
Artificial Neural Networks Approach of Data Analysis

- Artificial neural networks (ANN) is an universal tool for multidimensional approximation of experimental results.
- The Kolmogorov-Arnold theorem dealing with the capability of representation of multidimensional functions by means of superposition of functions of one variable is the basis of ANN application.

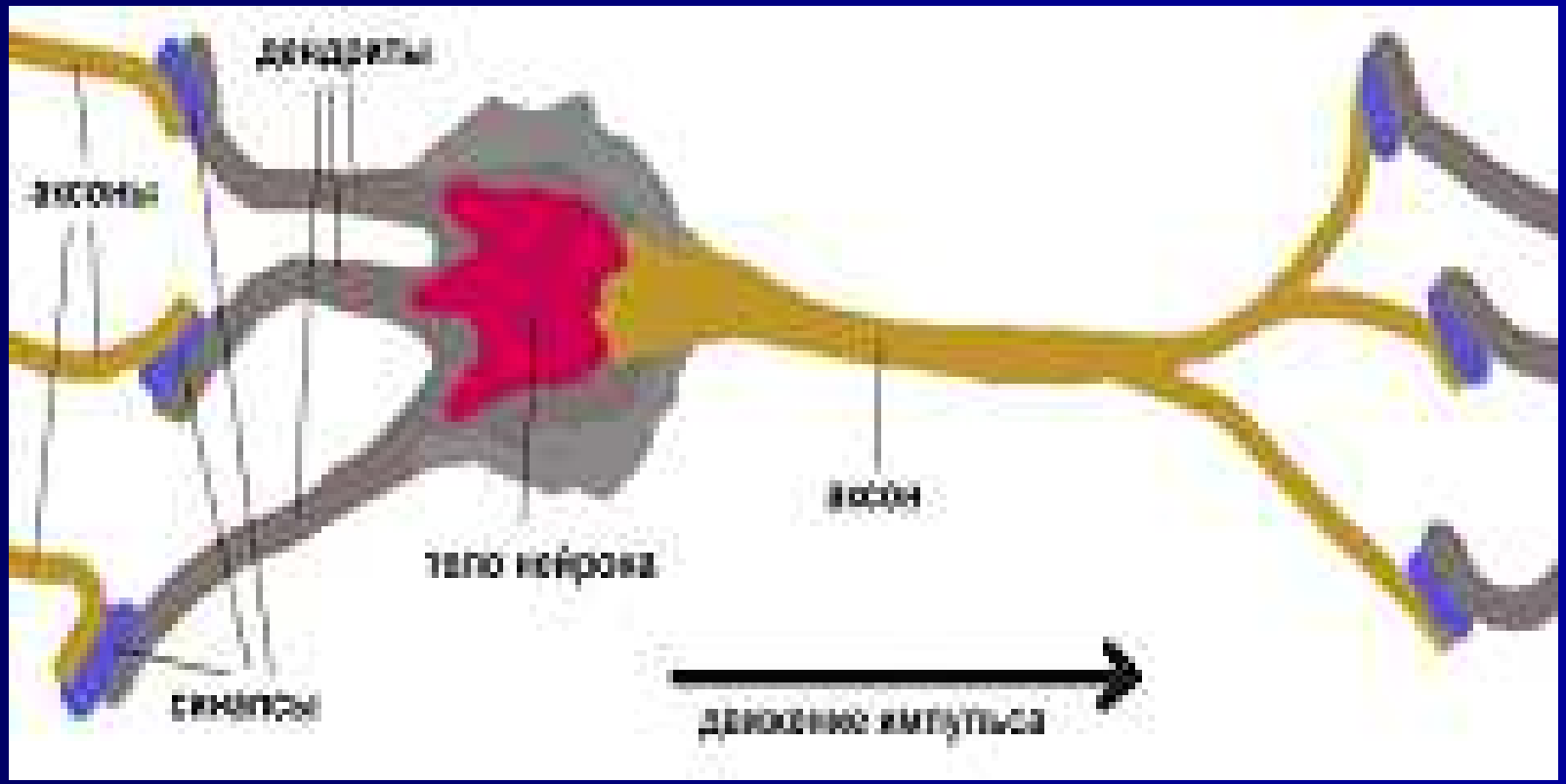
Artificial Neural Networks Approach of Data Analysis

- The real computer emulators of ANN are like the usual computer programs.
- The difference is that their creation is based on the use of a training procedure which executes by means of a set of examples (a data base of examples).
- ANN use principles of human brain working.
- They are like children and need in training

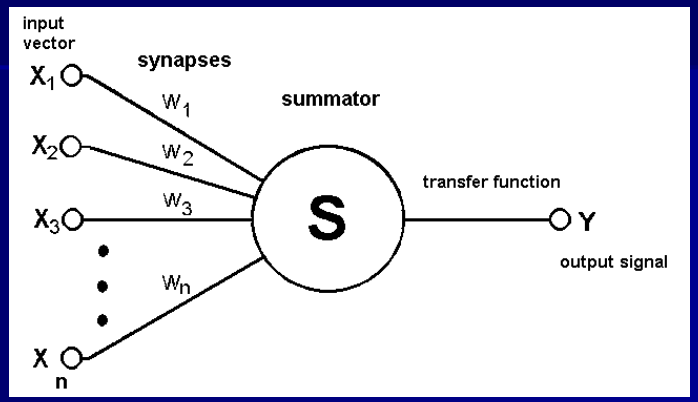
A part of human neural networks



Scheme of human neuron



Scheme of artificial neuron



Artificial neuron consist of inputs, synapses, summator and non-linear converter. It executes the following operations:

$$S = \sum_{i=1}^{n} X_i W_i$$

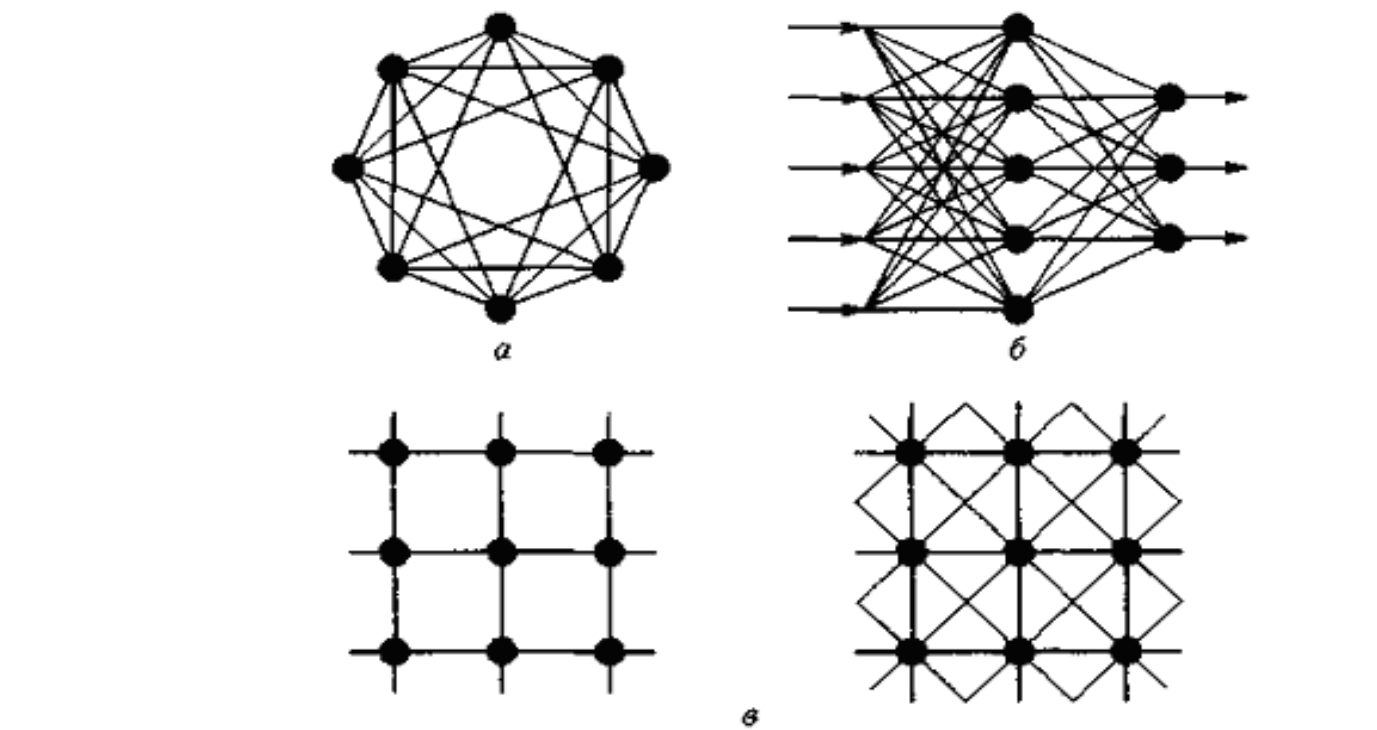
$$Y = f(S)$$

$$f(S) = \frac{1}{1+e^{-\alpha S}}$$

W i is the weight of a synapse (i = 1..., n); S is the result of summation; *Xi* is the component of input vector (input signals) (i = 1..., n); *Y* is the output signal of a neuron; *n* is the number of inputs of a neuron; and *f* is the non-linear transforming (function of activation or transfer function)

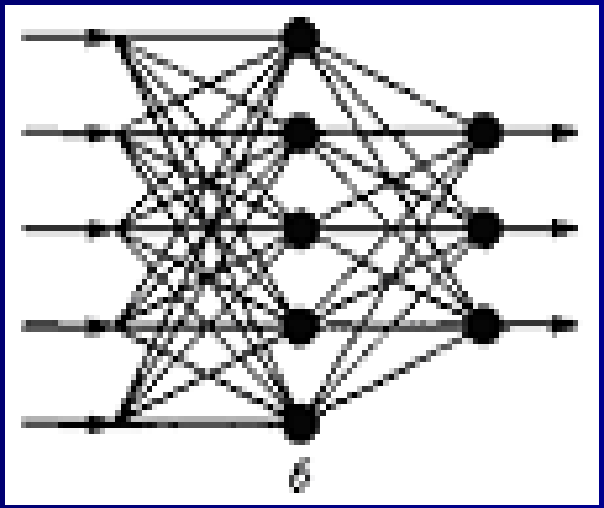
Kinds of Artificial Neural Networks

- ANN represent some quantity of artificial “neurons” and can be presented often as “neurons” formed in layers (б).



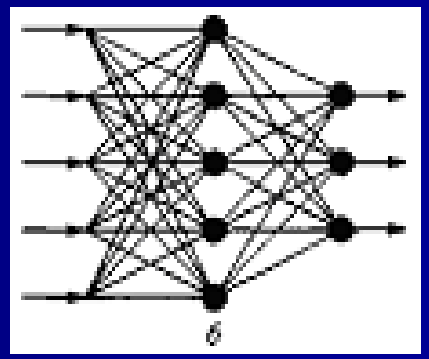
Example of Artificial Neural Networks

- A scheme of ANN which consists of one input layer, one "hidden" layer, and one output layer



Example of Artificial Neural Networks

- The input signals (five arrows on the left of Fig. are the input layer of neurons) go through synapses into the “hidden” layer of neurons (five black circles), then into the output layer of neurons (three black circles). Before and after passing the “hidden” layer, the input signals vary in accordance with the synaptic weight of each synapse of “neurons” of the “hidden” layer and their transfer function, as well as in accordance with the synaptic weight of each synapse of “neurons” of the output layer and their transfer function. The synaptic weight is a number which reflects a comparative contribution of each “neuron's” calculation into a final result (the output signals – three arrows on the right of Fig.)



Training of Artificial Neural Networks

- The task of ANN training consists of finding such synaptic weights by means of which input information (five input signals) will be correctly transformed into output information (three output signals). During ANN training, a training tool compares the output signals to known target values, calculates the error, modifies the weights of synapses that give the largest contribution to error by means of one of and repeats the training cycle many times until an acceptable output signal is achieved. A usual number of training cycles is more than 1000 …10,000. The concrete weights values obtained during training have no physical sense individually. However, the totality of them have a sense as a “black box” which allows for the transfer of any input signals belonging to the input signals used during training to a new output signal

Training of Artificial Neural Networks

- A database for ANN training can be formed by means of various techniques.
- An “art” of creation of a database is the first “art” of ANN technologies

Goal of the work

- There is a very important question: is it possible to predict what should be the nano material (structure, components, and dimensions) and what technology should be used with to provide the required properties and characteristics of nano materials?
- Here we present the results of application of ANN to create calculation models (CM) of a nano material and to look for answer the question.

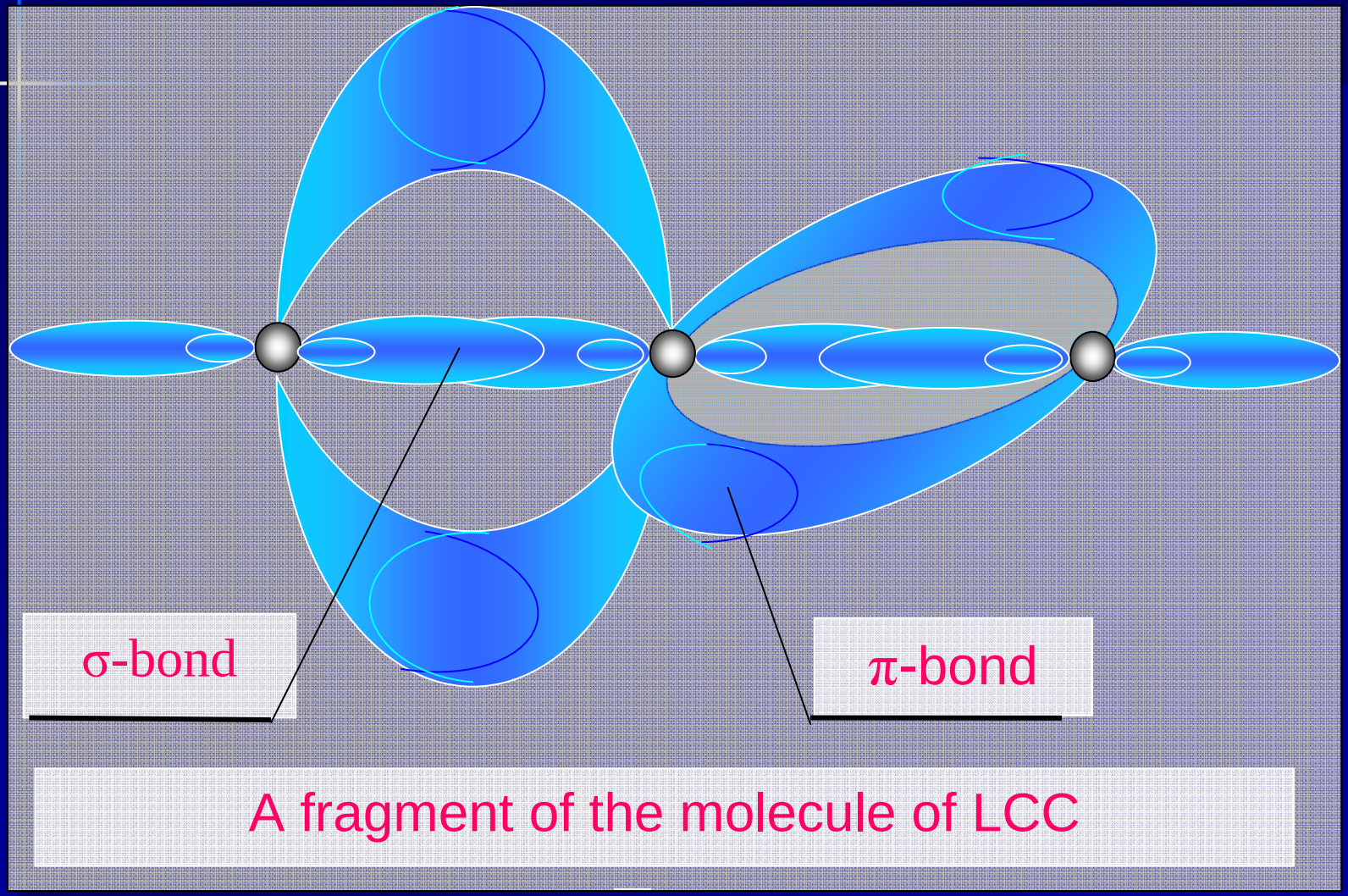
Examples of ANN usage for creation of calculation models (CM)

The CM are based on experimental results deal with characteristics of nano films of linear-chain carbon (LCC) with embedded into LCC metal and nonmetal atoms (LCC MNA).

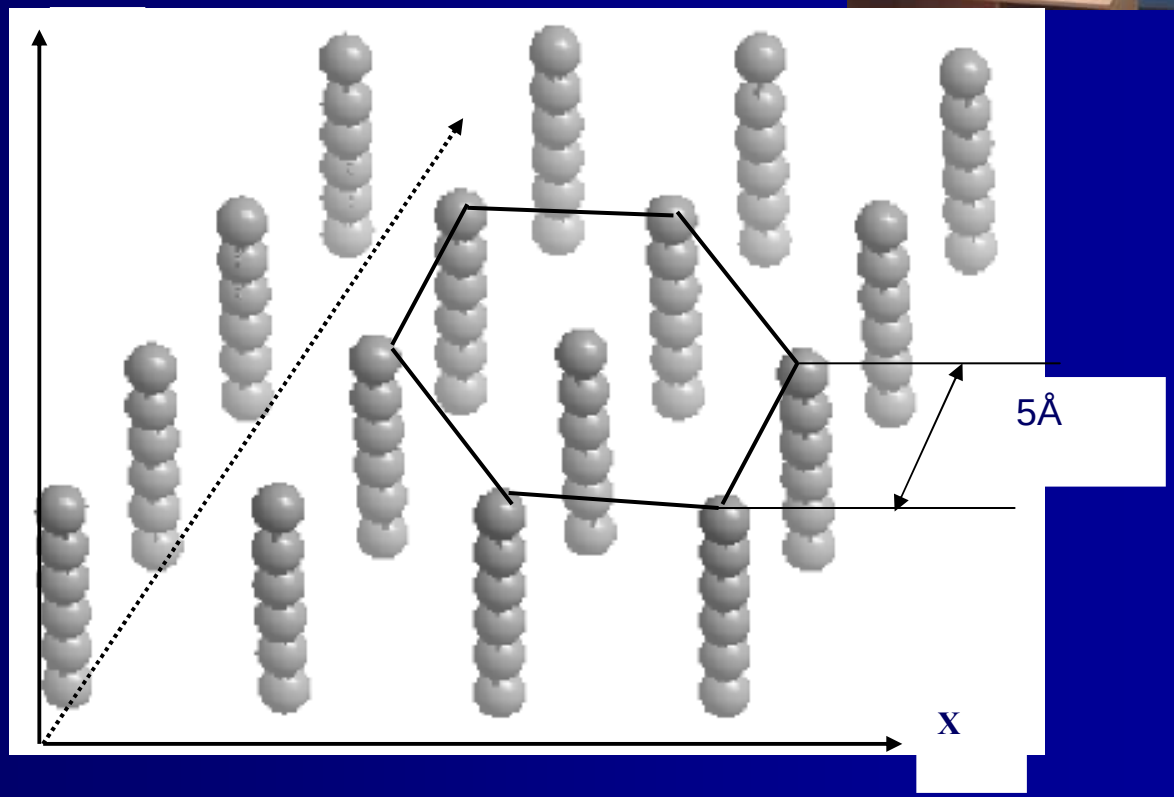
For the first time LCC MNA were manufactured in the Chuvash State University, using unique technology protected by a patent.

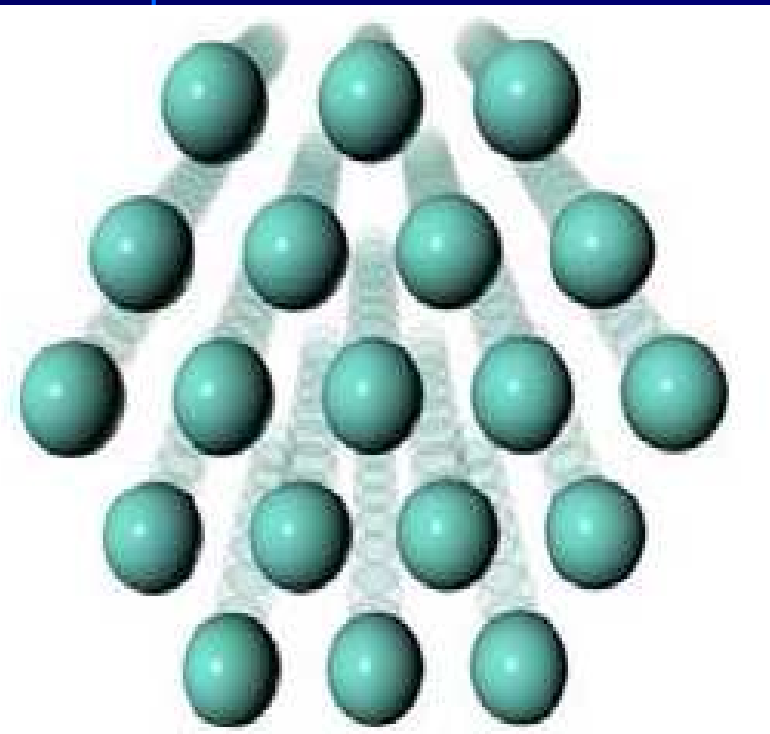
The direction of work can be of great interest for active and passive elements of solid-state electronics, sensors, medical applications, etc.

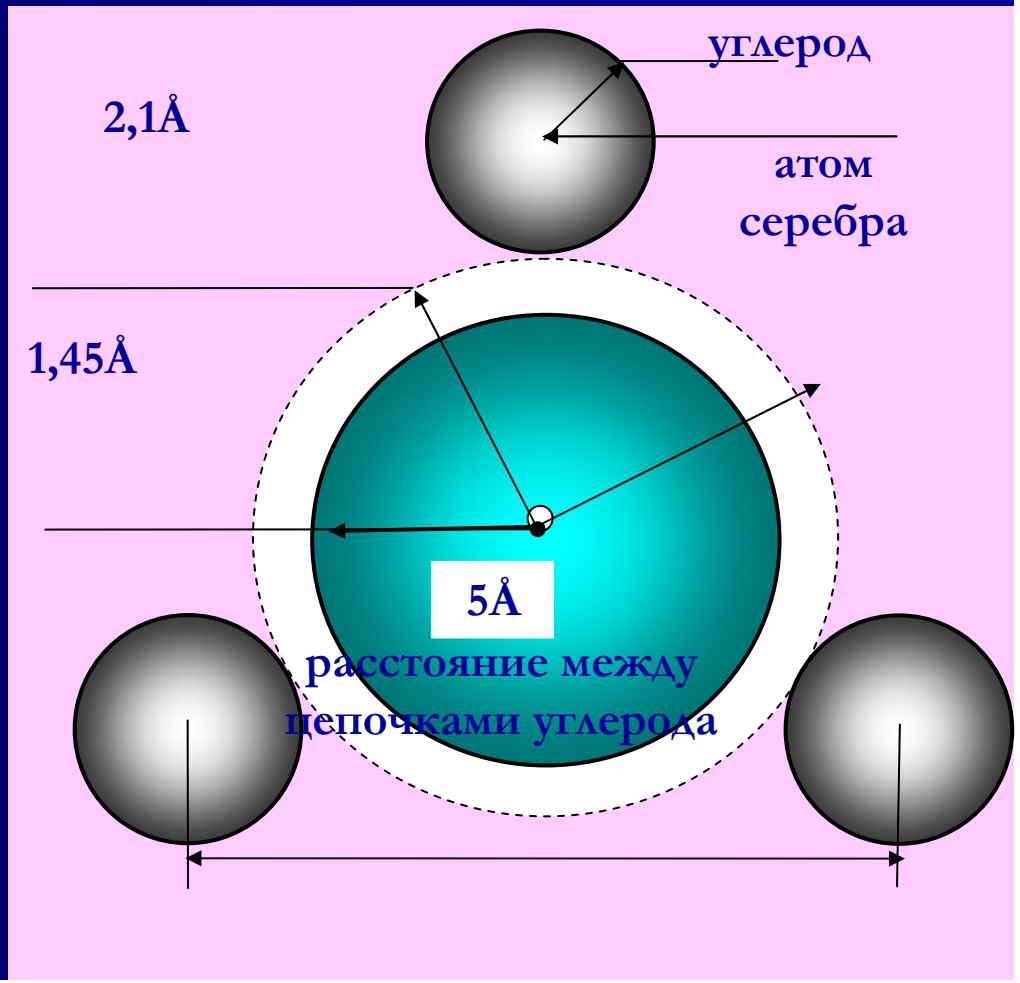
The electronic structure of the linear-chain carbon molecule



The film of line-chain carbon






углерод
2,1Å
атом
серебра
1,45Å
5Å
расстояние между
цепочками углерода

The model “Current-Voltage Characteristics of the LCC MNA”.

- The model allows us to predict the current-voltage characteristic of anything sort of LCC MNA.

The scheme of construction of the CM

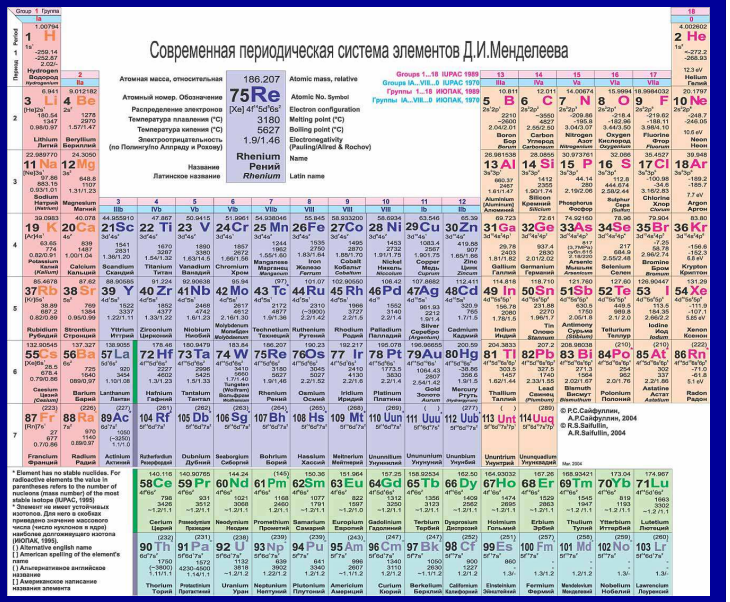
The scheme of construction of the CM was as follows.

- We have taken experimental data of the various type of LCC MNA

Part of experimental results used

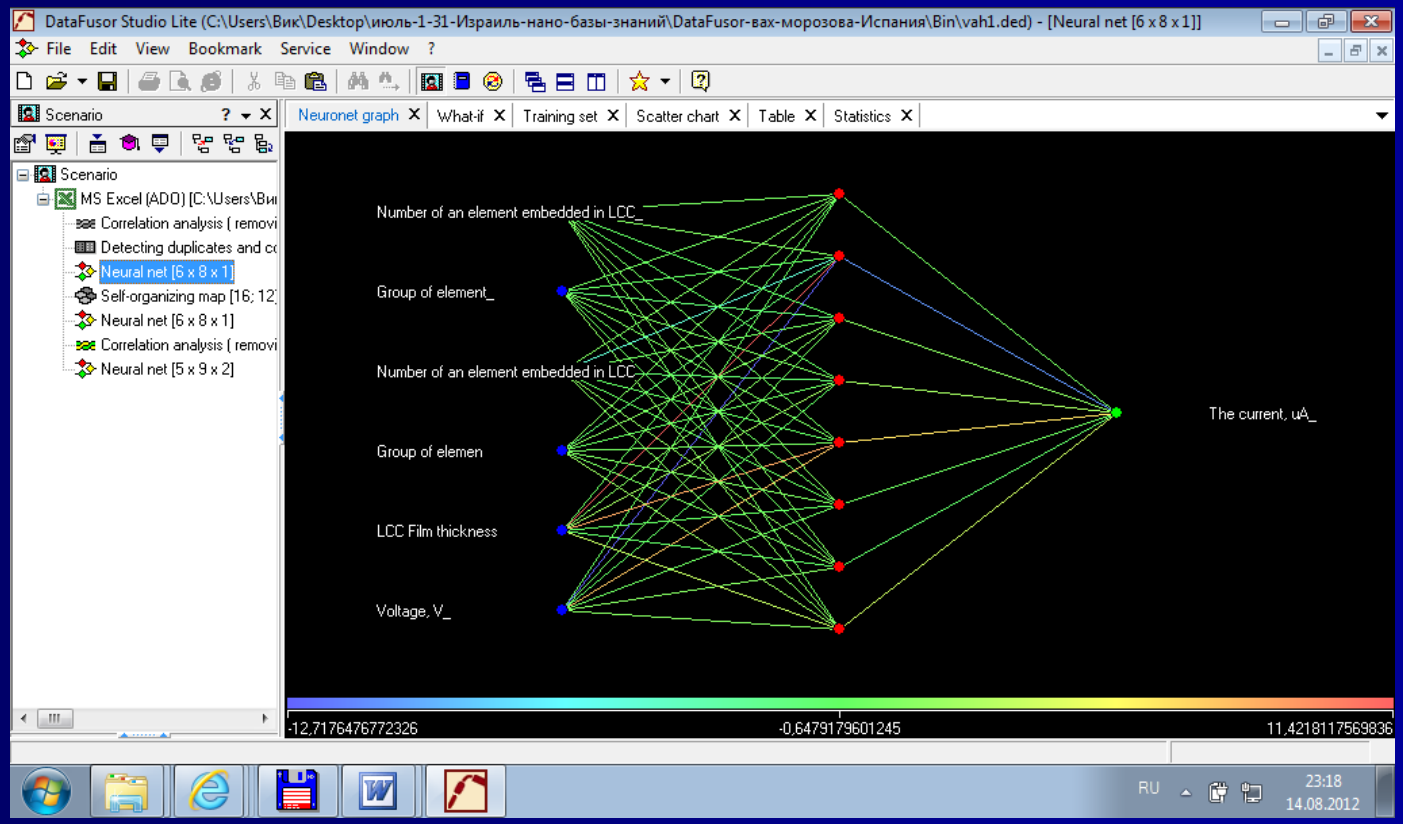
- In total, we had 150 rows which involved experimental data.

Number of an element1 embedded in LCC	Group of an element1	Number of an element2 embedded in LCC	Group of an element2	LCC Film thickness	Voltage, V	The current, uA
14	4	48	2	1000	2,9	-25,7
14	4	48	2	1000	-2,5	-23,8
…	…	…	…	…	…	…
14	4	48	2	1000	2,9	150,2
48	2	52	6	1000	-3,0	-7,5
48	2	52	6	1000	-2,8	-5,2
48	2	52	6	1000	-2,6	-3,5
…	…	…	…	…	…	…
48	2	52	6	1000	2,9	5,6
14	4	81	3	2000	-30	-50942,9
14	4	81	3	2000	-28,7	-36869,0
14	4	81	3	2000	-15,4	-3721,3
14	4	81	3	2000	-12,4	-2144,6
…	…	…	…	…	…	…



The structure of ANN

- Then we have chosen the structure of ANN in accordance with dimension of experimental data.



Training of ANN – getting of CM

- Then, the different sets of values of the first six column ((Number of an element1 embedded in LCC, Group of an element1, Number of an element2 embedded in LCC, Group of an element2, LCC Film thickness, Voltage (V)) were stored on the input layer of ANN. The corresponding values of the current (uA) were stored on the output layer of ANN
- By means of a training tool named the method of “back propagation of errors,” we have trained ANN and created CM. This model is a “black box” type

Training of ANN - getting of CM

Input values

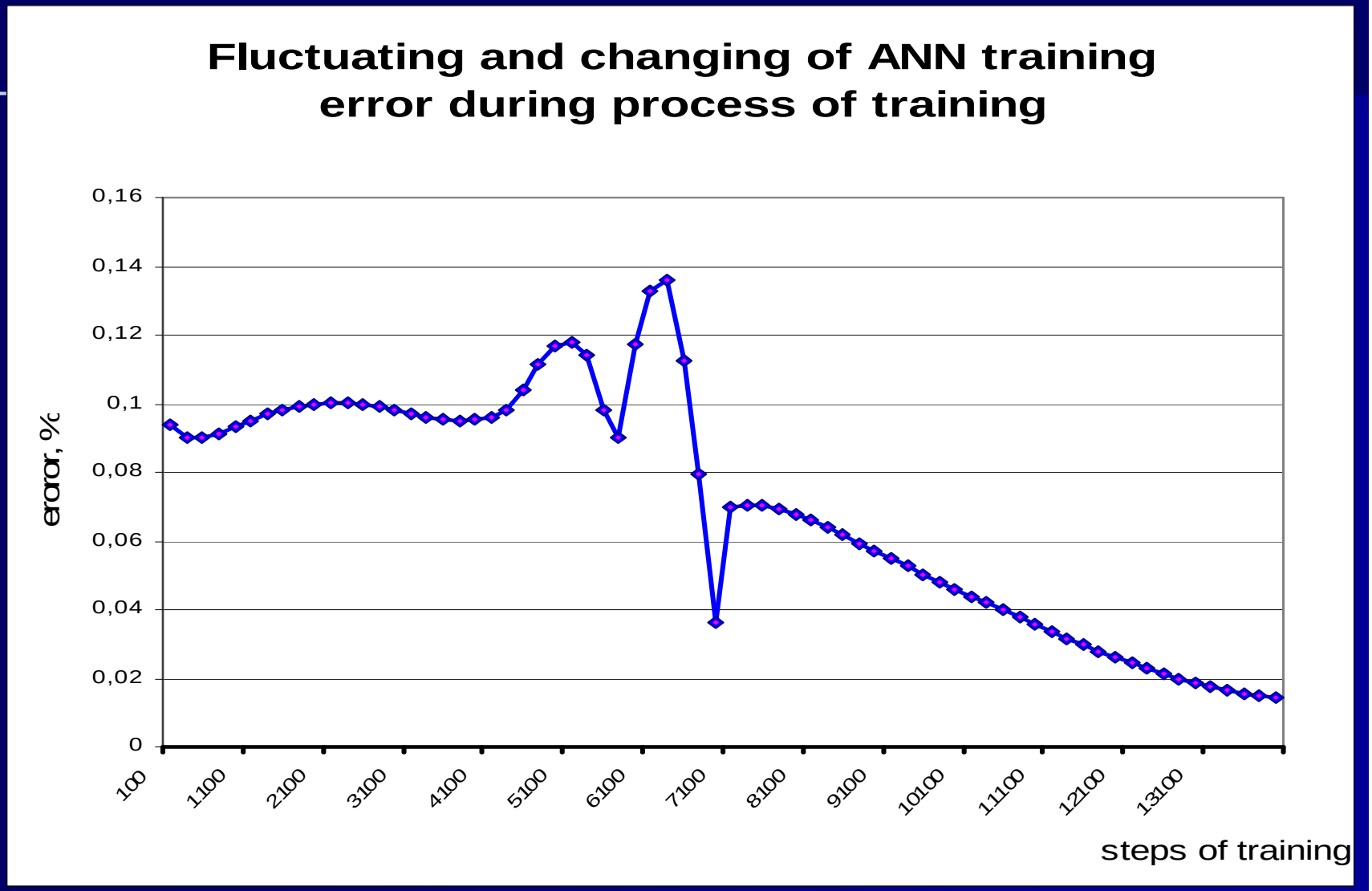
ANN

ANN (i, j, …)

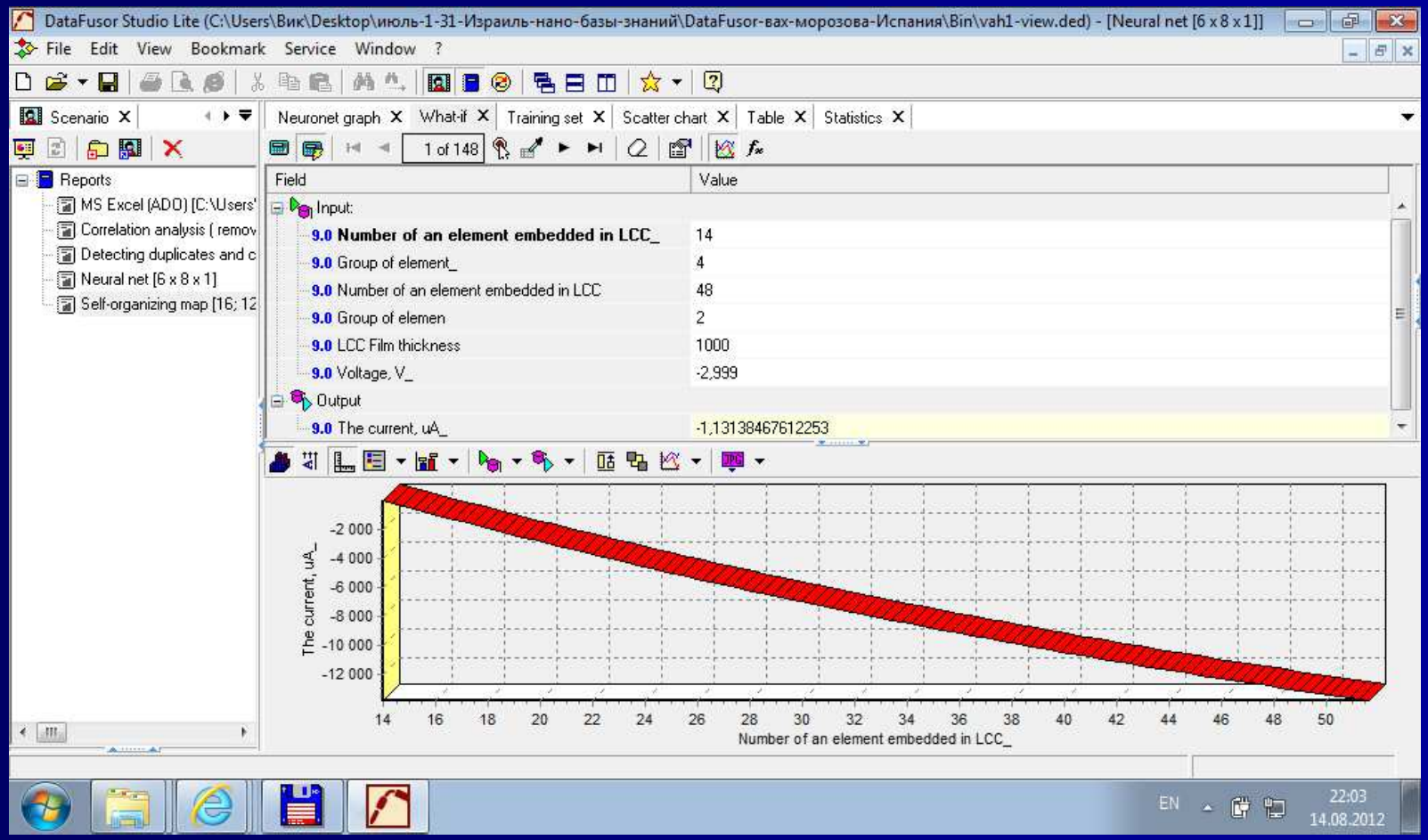
Output values

“back-prop”

“Back propagation of error”



The illustrations of dependences revealed by CM



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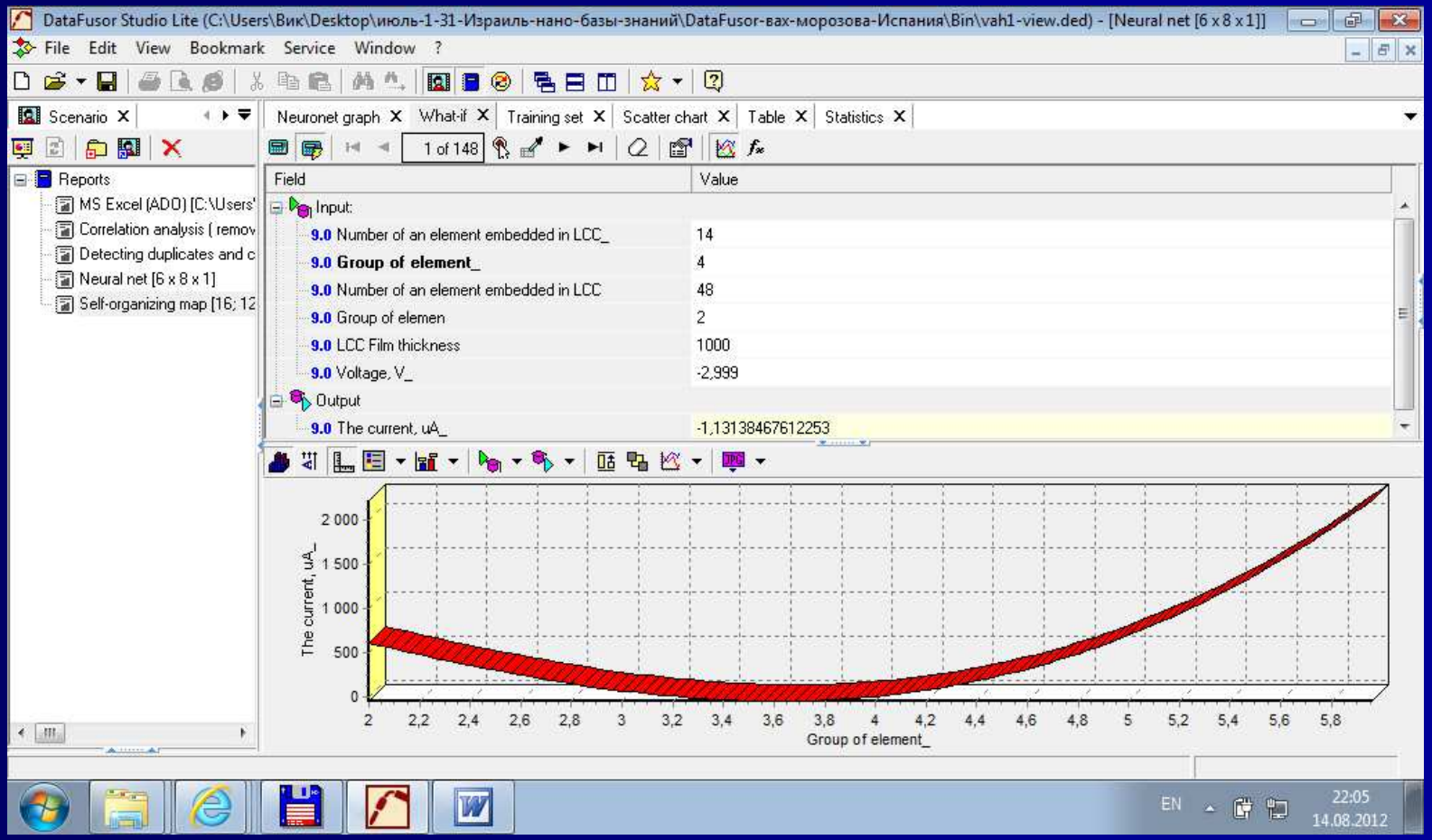

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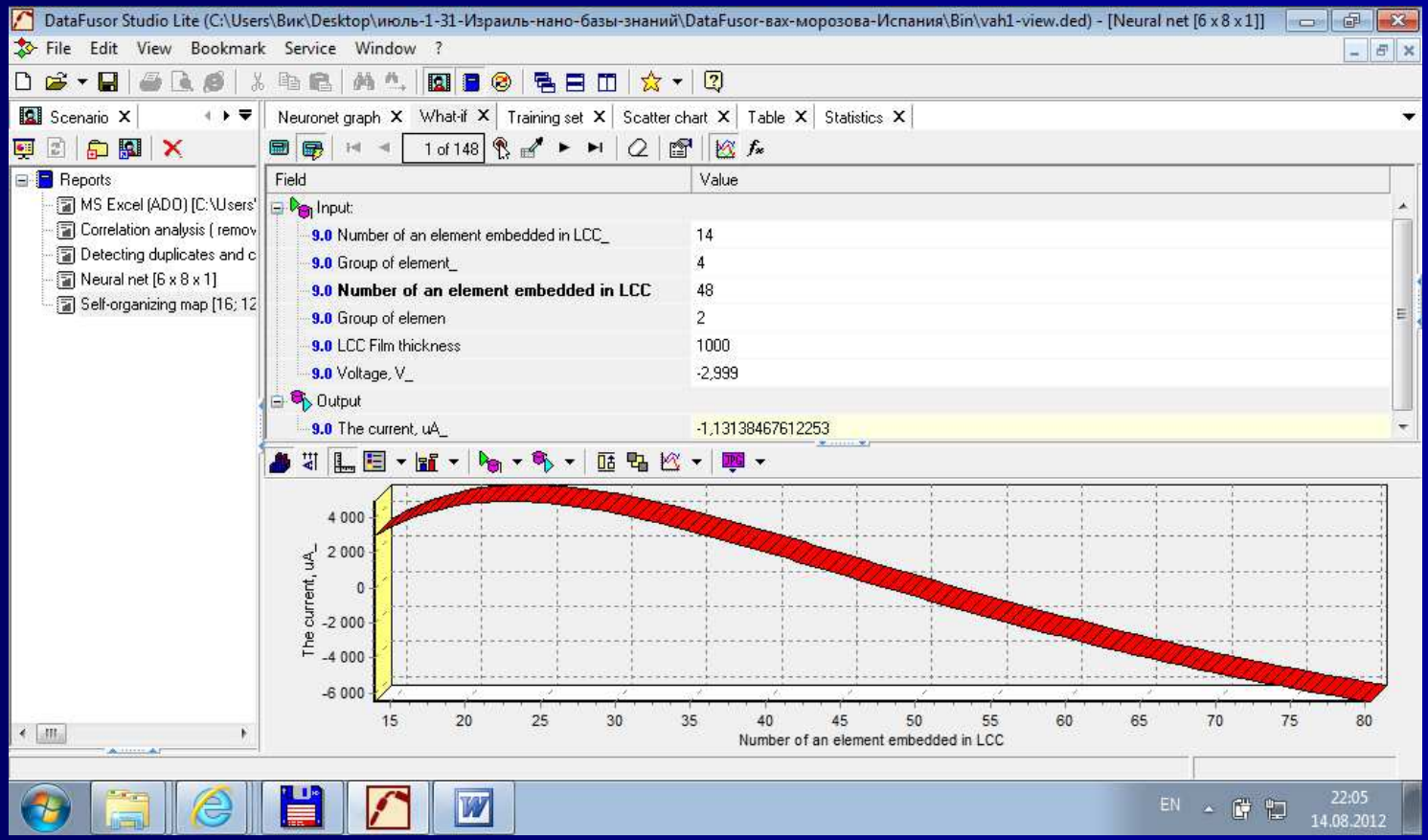

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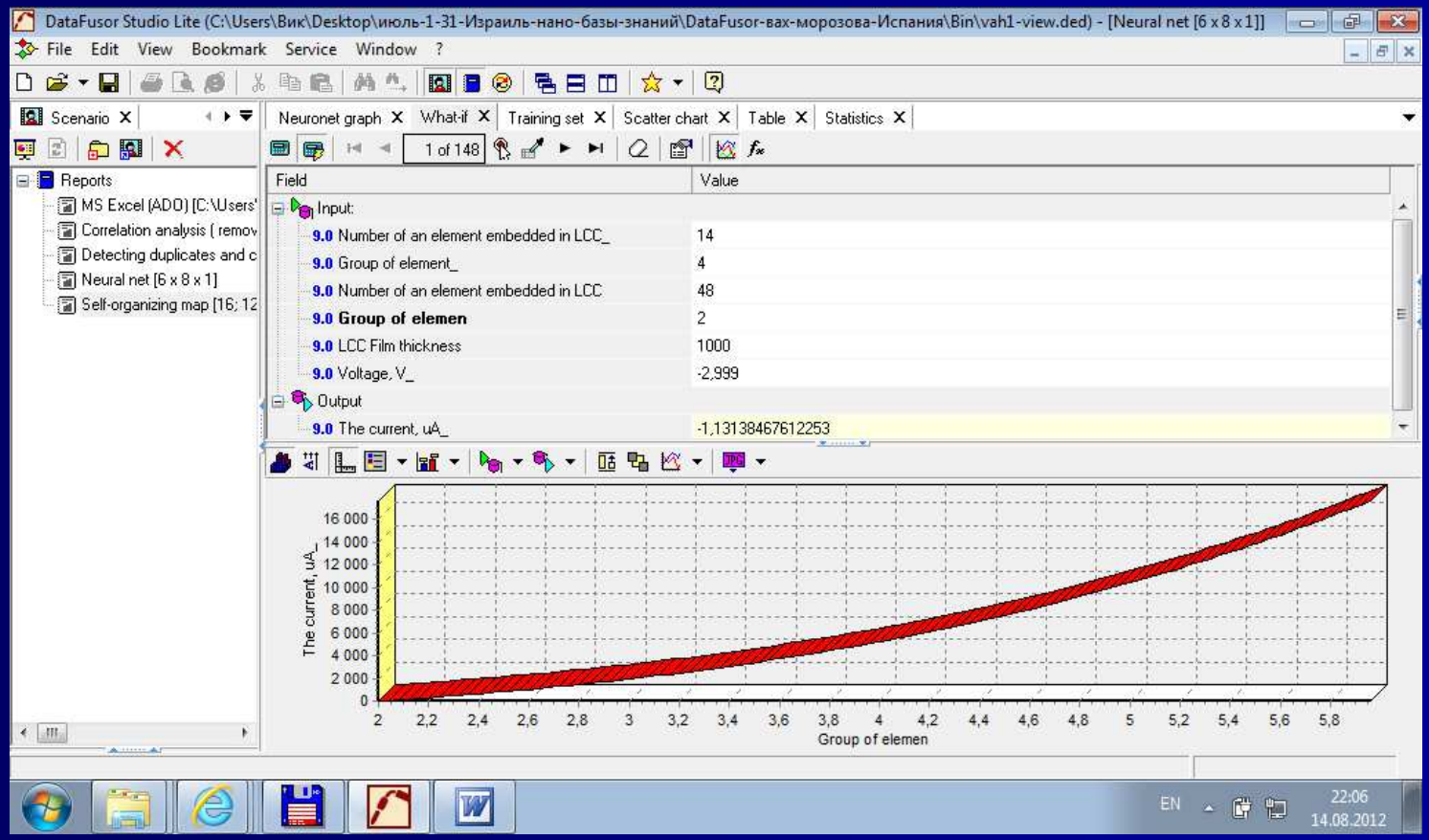

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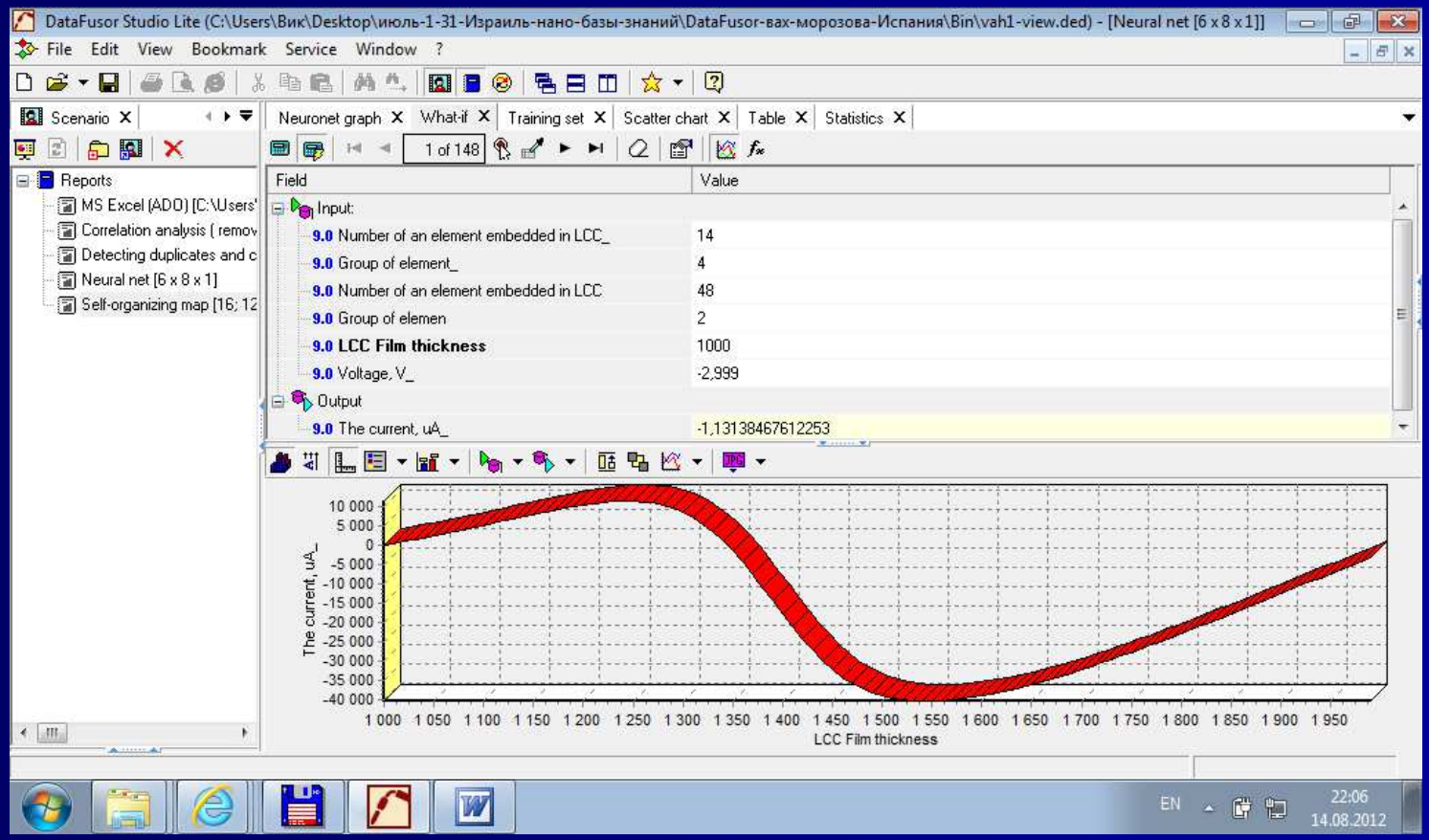

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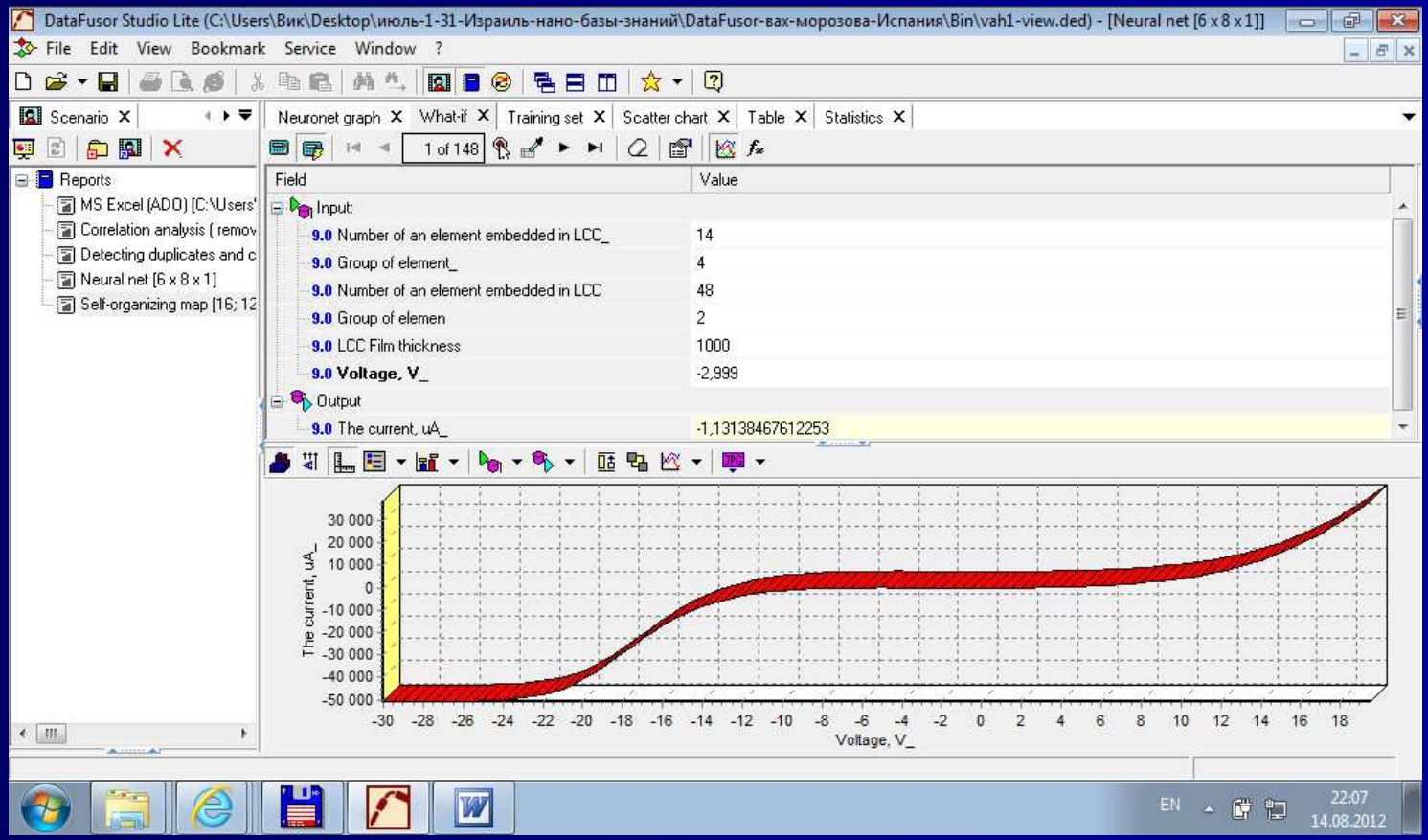
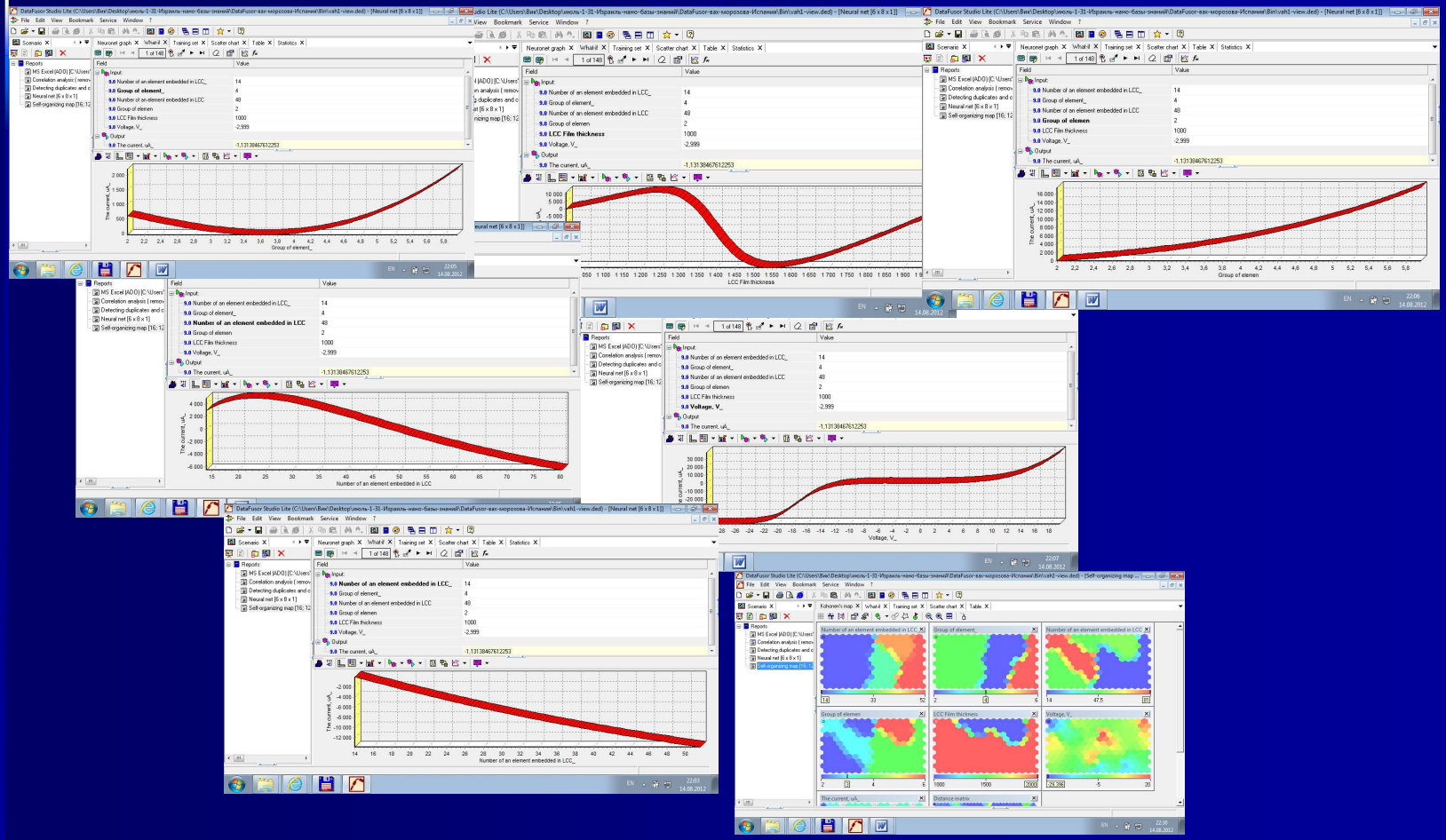


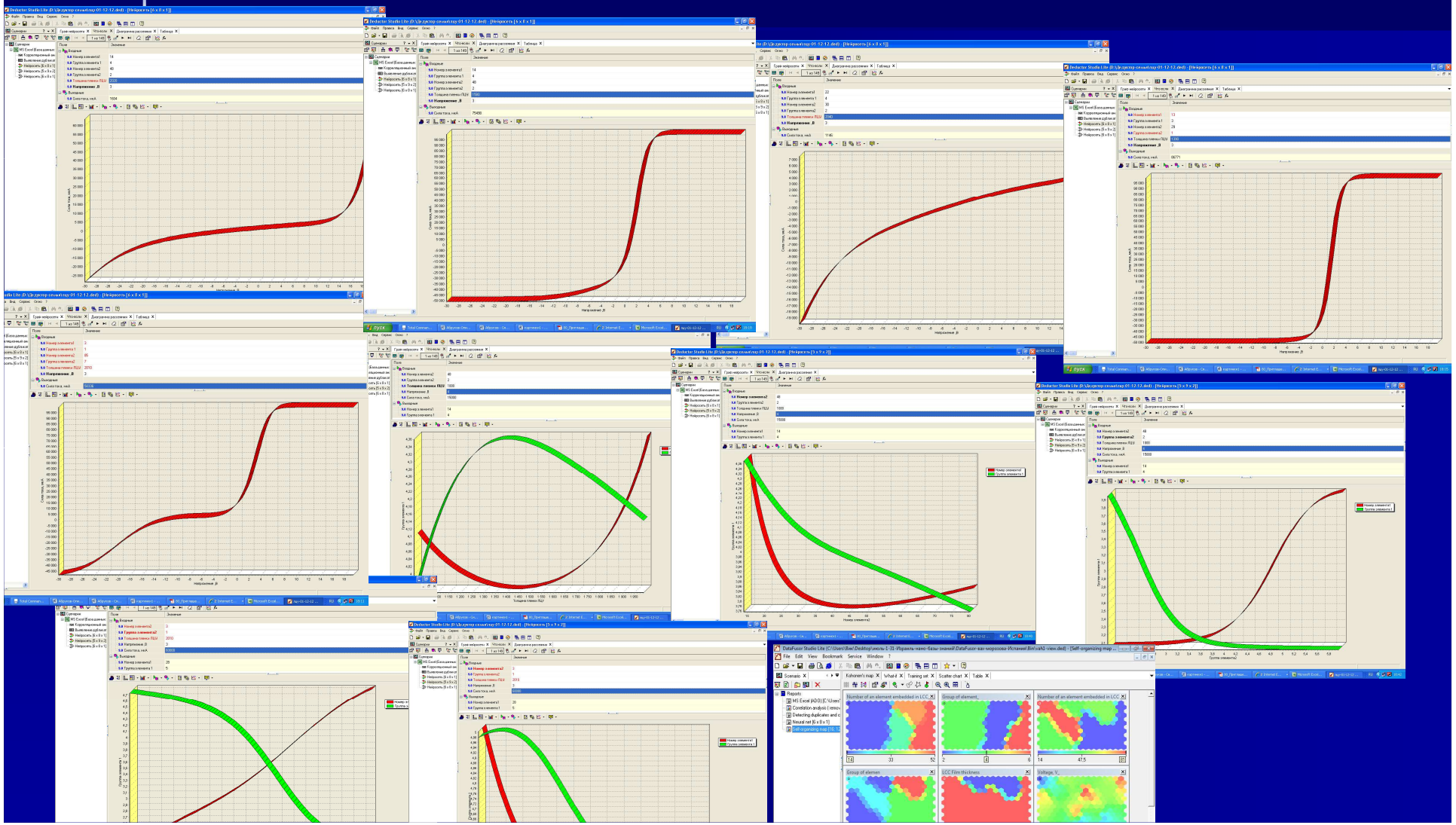
The illustrations of dependences revealed by CM

Only a little part of knowledge that there are in CM and can be obtained and illustrated instantly (in English):



The illustrations of dependences revealed by CM

Only a little part of knowledge that there are in CM and can be obtained and illustrated instantly (in Russian):



Outputs

An analysis of results obtained has depicted that:

1. The CM correctly “determines” the Current-Voltage Characteristics of LCC MNA and it is the good approximation tool of multidimensional experimental functions
2. The CM correctly reveals all dependences of the current on other parameters and it is the good tool for generalization and prediction of connection between variables.
3. The CM instantly calculates a value of the necessary characteristic and it is the fast engineering calculator specialized to LCC MNA
4. The CM easy gets any characteristics of a hypothetical sort of LCC MNA and it is the most cheap way for receiving of “new” “experimental” results without an experiment
5. The CM is The Knowledge Base of LCC MNA!

Conclusion

All you need in your life is love

All you need in your scientific life is neural networks

It can be artificial neural networks

One reference

1. **Neural Networks for Instrumentation, Measurement and Related Industrial Applications (2003).** ***Proceedings of the NATO Advanced Study Institute on Neural Networks for Instrumentation, Measurement, and Related Industrial Applications (9-20 October 2001, Crema, Italy)/*** **ed. by Sergey Ablameyko, Liviu Goras, Marco Gori and Vincenzo Piuri, IOS Press, Series 3: Computer and Systems Sciences – Vol. 185, Amsterdam.**