Nano films of linear-chain carbon with embedded metal and nonmetal atoms: Data Mining modeling

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Abstract

In this paper we aim to present a new nano material: nano films of linear-chain carbon with embedded metal and nonmetal atoms and results of its modelling by means of Data Mining tools. The embedding of atoms can fundamentally change the properties of the source material. The purpose of modelling is summarization of these changes and prediction what atoms should be embed in nano film of linear-chain carbon in order to modify its properties as desired.

1. Introduction

Currently a lot of experimental data on properties and characteristics of various nano materials are obtained in all of the world. The question is how we can summarize it and present in the form of common models that allow to describe the characteristics of previously studied nano materials? It is obvious that the characteristics of nano materials related to the composition of nano materials and type of components, manufacturing technology, the shape and size. The question is how we can generalize these links as computational models that allow determining the characteristics of the nano materials without carrying out additional experiments? Even more 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?

In this paper we present the first results of application of Data Mining (DM) [1], [2] to create such models. They are based on experimental results for the 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 [3], using unique technology protected by a patent [4], and using a variety of know-how. The direction of work can be of great interest for active and passive elements of solid-state electronics [5], sensors, medical applications, etc.

2. Methods of modelling

The Data Mining (DM) is a complex of contemporary tools for experimental (real and numerical) data pre-processing, processing, analysing, modelling and visualization. The DM involves such kinds of tools as various data pre-processing and processing tools (missing data recovery, fix abnormal values, finding duplicate and conflicting records, spectral processing), analysing tools (factor analysis, correlation and autocorrelation analysis, linear and logistic regression), modelling tools (decision trees, artificial neural networks (ANN), self-organisation maps - Kohonen maps, association rules, the user model). The ANN as universal tool for approximation of functions of several variables plays a major role in terms of a creation of computational models in order to generalize the experimental data and predict the properties and characteristics of nano materials. ANN are of most interest in computational mathematics and in many related scientific and applied research from the standpoint of a practical solution to multi-factor problems. However the other analysing and modelling tools have the important role too.

3. Results of Modelling

To date we have developed several computational models (ANN-models) that allow us to predict the physical-electrical properties of LCC MNA as a function of atoms embedded in a LCC, and the thickness of the film: 1. The model "Steepness and Saturation Current of the current-voltage characteristics vs. Kind of Embedded Chemical Elements". 2. Model "Steepness and Saturation Current of current-voltage characteristic vs. thickness of the film LCC. 3. Generalized model of "Current-Voltage Characteristics of the LCC MNA". The latter model allows us to predict the current-voltage characteristic of any new sort of LCC MNA. Examples of results obtained using the model 3 are depicted in Fig. 1.

Scheme for constructing models was as follows. Firstly experimental data of various LCC MNA current-voltage characteristics that we had were collected. Example of experimental data used is depicted in Table 1. The total number of rows actually used to construct the ANN model 3 was equal to 150.

Table 1

Example of data used to create the ANN model 3 of the current-voltage characteristics of LCC MNA films. Numbers and Groups of elements that are embedded in the LCC MNA are depicted in accordance with the numbers and groups in the Mendeleev's periodic table.

Number of an element embedded in LCC	Group of an element	Number of an element embedded in LCC	Group of an element	LCC Film thickness	Voltage, V	The current, uA
14	4	48	2	1000	2,999	-25,751
14	4	48	2	1000	-2,515	-23,874
…	…	…	…	…	…	…
14	4	48	2	1000	2,94	150,23
48	2	52	6	1000	-3,01	-7,548
48	2	52	6	1000	-2,879	-5,202
48	2	52	6	1000	-2,636	-3,52
…	…	…	…	…	…	…
48	2	52	6	1000	2,934	5,67
14	4	81	3	2000	-30	-50942,98
14	4	81	3	2000	-28,79	-36869,05
14	4	81	3	2000	-15,454	-3721,339
14	4	81	3	2000	-12,42	-2144,635
…	…	…	…	…	…	…

The task of modelling is the task of approximating of the experimental function of six variables.

After choosing the architecture of ANN relevant to collected data base (Table 1), we held ANN "training". During training the different sets of values of the first six columns of Table 1 were installed to the input layer of ANN, and the corresponding values of current were installed in the output layer of ANN, and using a well-known method of ANN training - a method of "back propagation of errors" [1] we created a computer ANN model of current-voltage characteristics (computer emulator of ANN).

This model is a model of the "black box" type. The resulting "black box" can be used to determine (predict) the current-voltage characteristics of the LCC MNA for different combinations of kinds of chemical elements embedded in the LCC MNA without carrying out experiments as follows. The number of group of the element in Mendeleev's periodic table and the number of element as well as the thickness of the LCC MNA and a voltage value install in the input layer of the computer-ANN model. After that the "black box" instantly calculates corresponding to this data set the current value as well as (!) the current-voltage characteristics as a whole.

An example of the results is depicted in Fig. 1.

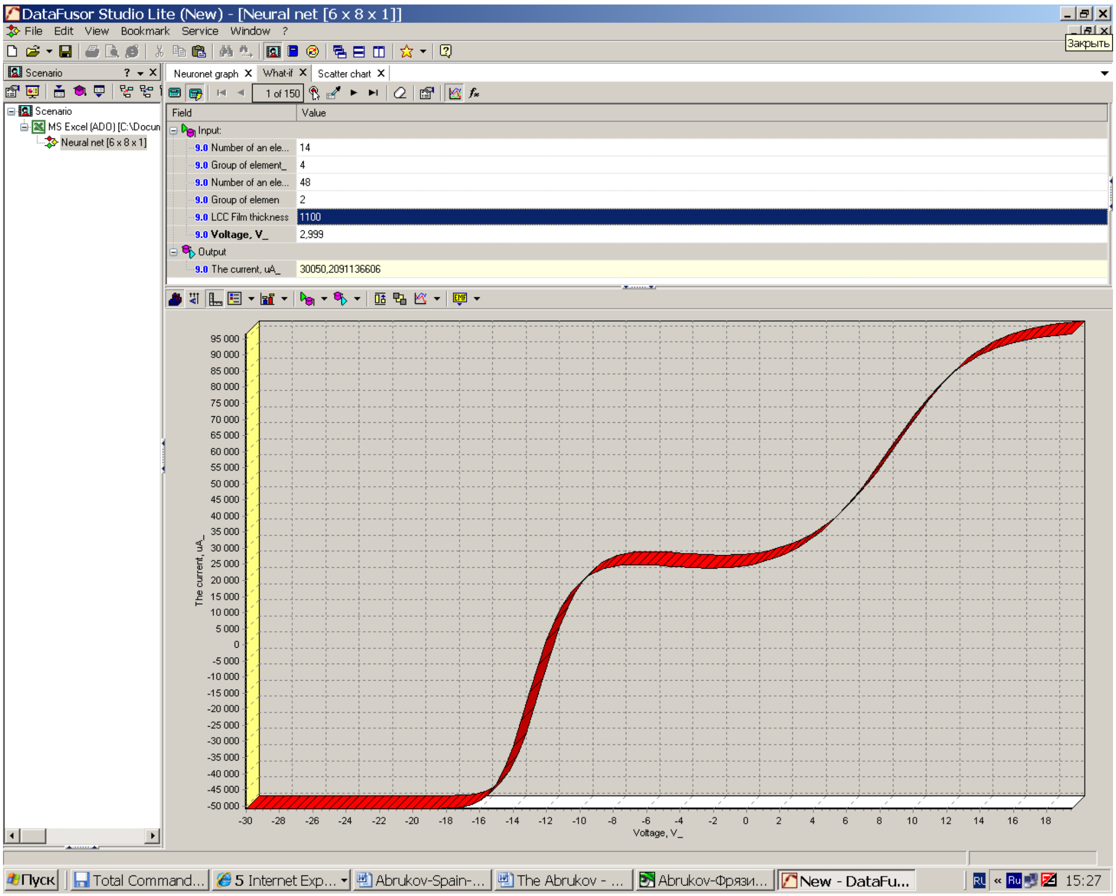

Fig. 1. Approximation of the current-voltage characteristics of the LCC MNA with embedded silicon and cadmium atoms into the film with the thickness of 1100 angstroms.

4. Conclusion

We believe that the Data Mining tools in particular the ANN are very promising methods of analyzing the available experimental results. They allow summarize the experimental results in a qualitatively new level (in the form of a computational model) and thereby significantly increase their value as well as they allow to obtain (to predict) the new "experimental" results without direct experimentation.

References

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