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A new material experiment: Data mining for modeling, data mining for presentation

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Questions and Problems:

What does it mean that you have completed the material experiment? This means that you have tables and graphs.

The main question that we want to put is how can you increase the significance (profit, price) of the tables and graphs that you have received?

For example:

How can you generalize them? How can you use them to solve the inverse problem?

Other questions:

How can you go beyond the experiment that you have completed?

How can you go outside the tables and graphs? How far?

Can you predict the results of experiments in the area of your research that you were not being able to execute? How accurately can you predict them?

Data Mining:

In the work we present the examples of the Data Mining (DM) usage for solution of these questions and problems.

DM involves tools such as decision trees, artificial neural networks (ANN), self-organization maps, etc. ANN plays a leading role for a creation of multifactor computational models. We have an analytical platform that includes preparation of data, selection of informative indicators, data cleansing, and use of ANN to create the multifactor computational models. ANN can be considered a universal tool for approximation of experimental function of several variables. The Kolmogorov-Arnold theorem, which deals with the capability of representation of a function of several variables by means of superposition of functions of a smaller number of variables, is the basis of ANN applications. We present the multifactor computational models of the characteristics of nano films of linear-chain carbon (LCC) (carbene) with embedded into LCC various atoms (LCCA) that depict how we solve these questions and problems. For the first time LCCA were manufactured in the Chuvash State University, using unique technology protected by a patent, 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, photovoltaic elements, sensors, medical applications, etc.

We will present two ANN-models that allow us to reveal all dependences between variables, to generalize them, and to calculate the physical-electrical and optical properties of LCCA in dependence on amount of kind of atoms (one or two kinds) embedded in a LCCA, kind of atoms (number and group of atom in accordance with the Mendeleev's periodic table), and the thickness of the LCCA: 1. The model of "Current-Voltage Characteristics of the LCCA", 2. The model of "Transmission coefficient spectrum of the LCCA". The models allow us to predict the current-voltage characteristic and transmittance spectrum of any new sort of LCCA with any atoms of the Mendeleev's periodic table. The models allow also to solve an inverse task: to determine the amount of kind of atoms, the kind of atoms, and the thickness of the LCCA that provide a required a current-voltage characteristics and a transmission coefficient spectrum of LCCA. We invite participants of MSE-2013 who are interested in the creation of the multifactor computational models in the area of materials science to collaborate with our team. If you have a table of experimental data in the format of MS Excel or Windows txt file we can create the ANN multifactor computational model of your data during 5 …10 minutes.

Data Presentation:

Data mining gives to the experiment a new quality. This allows give a new quality to the presentation of experimental data in the articles for scientific journals. We believe that it is necessary to introduce the following change in the representation of experimental research in scientific journals. It is necessary to enter a recommendation to submit as an annex to the paper a computer copy of the model obtained by using artificial neural networks. This model will allow the reader to get the most complete picture of the experimental work. It allow to a reader itself to solve all issues and problems that were set at the beginning of our work.

Biography

Victor S. Abrukov has completed his Dr. of Sci. at the age of 43 years from the Semenov Institute of Chemical Physics of the Russian Academy of Science. He is the Professor at Chuvash State University since 1996, Head of Department of Thermal Physics (1996 to 2012) and Department of Applied Physics and Nanotechnology (2012 to now) at the Chuvash State University. He has published more than 60 papers in reputed journals.

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