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Knowledge base is a future of nanomaterials world

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Abstract

Modelling is still emerging to become the key for industrial progress in areas ranging from materials research to the development of novel and improved applications.

Currently a lot of experimental data on properties and characteristics of various nanomaterials are obtained in the entire world. The question is how we can summarize it and present in the form of common models allowing description the characteristics of previously studied nanomaterials?

It is obvious that the characteristics of nanomaterials related to the composition of nanomaterials and type of components, manufacturing technology, the shape and size. The question is how we can generalize these links as computational models (CM) that allow determining the characteristics of the nanomaterials without carrying out additional experiments?

Even more important question is it possible to predict what should be the nanomaterial (structure, components, and dimensions) and what technology should be used with to provide the required properties and characteristics of nanomaterials?

The Data Mining (DM) is a complex of contemporary tools for experimental data pre-processing, processing, analysing, and modelling. 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 several variables experimental functions plays a major role in terms of a creation of CM in order to generalize the experimental data and predict the properties and characteristics of nanomaterials.

To date we have developed two CM (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 LCC MNA: 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 LCC MNA. The models allow us also to solve an inverse task: to determine what amount of kind of atoms, what kind of atoms, and what the thickness of the LCC MNA should be to provide the required "Current-Voltage Characteristics" and "Transmission coefficient spectrum" of LCC MNA.

We present an example of the results of application of Data Mining (DM) in particular artificial neural networks (ANN) to create such CM. They are based on experimental results for the characteristics of nanofilms of linear-chain carbon (LCC) (carbine) with embedded into LCC various atoms (LCCA). 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.

Outputs: An analysis of results obtained has depicted that:

1. The CM correctly "determines" the Current-Voltage Characteristics and Transmission Coefficient Spectrum of LCCA and it is the good approximation tool of multidimensional experimental functions.

2. The CM correctly reveals all dependences of the current and transmission coefficient 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 LCCA and it is the most cheap way for receiving of "new" "experimental" results without an experiment.
5. The CM illustrates vividly all dependences and it is a good tool for presentation of experimental results obtained.
6. The CM obtained is the Knowledge Base of LCCA as well as prototype of a future Knowledge Base of nanomaterials world.

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