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OF DISCRETE DEVICES
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Настоящий том содержит полные тексты докладов, представленные на секциях «Высокоуровневое проектирование» и «Схемотехническое, топологическое и физическое проектирование» Шестой Международной конференции «Автоматизация проектирования дискретных систем» (Computer-Aided Design of Discrete Devices – CAD DD'07), Минск, 14–15 ноября 2007 г., в которых рассматриваются проблемы, возникающие на начальном и заключительных этапах проектирования цифровых устройств и сверхбольших интегральных схем.

Доклады напечатаны в виде, представленном авторами, и адресованы специалистам в области автоматизации проектирования дискретных систем.

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Материалы Шестой Международной конференции

АВТОМАТИЗАЦИЯ ПРОЕКТИРОВАНИЯ ДИСКРЕТНЫХ СИСТЕМ CAD DD'07

Том 1

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COMPUTER-AIDED DESIGN OF NEW INORGANIC COMPOUNDS PROMISING FOR SEARCH FOR ELECTRONIC MATERIALS

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The principles of computer-aided design of new inorganic materials promising for application to electronics are discussed. They are based on the use of computer analysis of information of databases on known inorganic substance and material properties. The methods of pattern recognition are used for computer analysis. Data analysis allows a search for regularities between the properties of substances and chemical elements forming these substances. Owing to periodicity of chemical element properties the extrapolation and interpolation of discovered regularities allow a prediction of new substances, not yet synthesized. The results of predicting new inorganic compounds promising for electronic applications are considered.

Introduction

Currently, automated design uses only data on properties of already known materials. For this purpose numerous databases (DB) on properties of materials and appropriate systems of a search and selection of existing materials are developed. Most prominent examples are the approach developed by M.Ashby and the computer system of material selection CES EduPack that was created on its basis [1]. However a large number of parameters of the existing materials do not satisfy the designers and thus limit capabilities of projected machines, buildings, devices, etc. In such dynamically developing branch of modern technologies as electronics and areas, associated with it, the traditional materials do not always provide a realization of necessary parameters of devices. Traditional methods of computer-aided design, for example, of VLSI [2], are focused on a standard set of used materials and do not assume any use of new substances. In this connection the idea of computer-aided design of new, not yet produced, materials with given parameters, is of much current interest.

1. Formulation of Problem

It is possible to divide the problem of design of new materials into two parts [3]: (1) searching for new substances with predefined properties and (2) development of optimum conditions for the production and treatment of new materials. The present paper is devoted, for the most part, to solution of the first problem of design of new inorganic compounds. This problem can be formulated as follows [4]: it is necessary to find a combination of chemical elements and their ratio (that is, qualitative and quantitative composition) for making (under the given conditions) the predefined space molecular or crystal structure of compound allowing a realization of necessary functional properties. Only properties of chemical elements and data about other already investigated compounds should be used as initial information for calculations. Thus, the problem is associated with a search for regularities between properties of chemical systems (for example, properties of compounds) and

properties of chemical elements which form these systems. Design of inorganic compounds is similar to traditional design of machines, devices, buildings: it is necessary to develop some structure from elements.

Examples of tasks of design in the inorganic chemistry and materials science are:

- the design of systems with compound formation or non-formation;
- the design of chemical systems with formation of compounds of desired composition at the predefined conditions;
- the design of inorganic compounds with a specific crystal structure type at the predefined conditions;
- the design of inorganic compounds with the predefined functional properties (critical temperature of transition to the superconducting state, band gap, melting point, and so on).

2. Methods of Solution of Problems

Current methods for inorganic substance design (quantum-mechanical and simplest empirical criteria) are not always efficient to solve these problems. Therefore the pioneering investigations of Baikov Institute of the sixties on application of computer-aided compound design [5, 6] have become as big break in inorganic chemistry and materials science. Researchers of Baikov Institute used by methods of pattern recognition for design of new, not yet synthesized, substances. Thousands of new compounds and their properties in binary, ternary, quaternary and more complicated systems were predicted using this approach [3-7]. The comparison of results of predicting with new experimental data shows that average reliability of their predictions exceeds 80 %.

In the case of application of pattern recognition methods it is possible to connect some discrete parameters of inorganic compounds (for example, possibility of formation of compound or type of its crystal structure under normal conditions) with properties of chemical elements, which are included into their composition, and also to get estimation of some numerical properties (for example, melting point of compound at atmospheric pressure, critical temperature of transition to superconducting state, etc.) [3-8]. It is important, that the fulfillment (though also not so strict) of basic hypothesis of methods of pattern recognition - hypothesis of compactness - is a consequence of the Periodic Law. Each compound corresponds to a point in multi-dimensional space of properties of elements. Owing to periodicity of properties of chemical elements points, which correspond to combinations of close with properties elements, combining into compounds, form compact clusters. Thus, the task of search for regularities connecting property of inorganic compounds with properties of chemical elements can be reduced to a problem of computer learning in pattern recognition. In this case the analysis of the information about already known compounds, which are represented as a set of values of properties of chemical elements, allows a discovery of classifying regularities. The latter allow a separation of known compounds into predetermined classes. It is possible to predict new compounds and estimate their unknown parameters by substitution of the property values of the appropriate chemical elements into the found regularities.

The principal problems at application of methods of pattern recognition to the decision of tasks of inorganic chemistry are following:

1) small informativeness of attributes - properties of chemical elements;
2) the strong correlation of these attributes owing to their dependence on common parameter - atomic number of chemical elements (it follows from the Periodic Law);
3) omissions in values of attributes;
4) in many cases - the large asymmetry of a size of classes of training set;
5) sometimes feature description includes non-numerical attributes;

6) possibility of experimental mistakes of classification in training sets.

Therefore we have tried to choose methods of pattern recognition, which would be the best for solution of the problems mentioned above. We tested various algorithms in our investigations: ConFor [10], *k*–nearest neighbors, Fisher's linear discriminant, linear machine, neural networks, genetic algorithm, estimates calculation algorithms, deadlock test algorithm, statistical weighted syndromes [11], support vector machine [8, 11], etc. [11, 12]. It was established during testing various algorithms of computer learning for some tasks that it is impossible to specify beforehand, what algorithm is most effective at the decision of the certain chemical task of design of inorganic compounds. Quite often programs, which have classified training set well, obtained bad results at the prediction of unknown compounds. In this connection the most effective way of decision of tasks of predicting properties of new inorganic compounds is associated with methods of recognition by collectives of algorithms [11]. At synthesis of the collective decision it is possible to compensate mistakes of separate algorithms by the correct predictions of other algorithms.

3. Example of Computer-Aided Design of Compounds Promising for Search for New Materials for Optoelectronics

The chalcopyrites with composition ABX_2 are class of compounds that are promising for the development of new semiconducting [13-17], nonlinear optical [14, 15, 17-19], and other materials for electronics. The aim of our investigations was to design new semiconducting compounds with crystal structure of chalcopyrite and band gap more than 2 eV for development of optoelectronic devices. Recent developments in optoelectronics and other fields of practical applications (in particular, high-temperature devices and methods of detecting photons and charged particles) have stimulated an interest in wide band gap semiconductors [20].

Earlier we had predicted the new chalcopyrites [7] and estimated melting point and band gap of known compounds with this crystal structure [9]. Now using the systems RECOGNITION [11], ConFor [10], MASTER [8] and attribute selection/weighting methods [12] we tried to predict new chalcopyrites of composition ABX_2 (A, B and X – various chemical elements) and to estimate a band gap of new compounds. In the last case our approach makes possible evaluating value of property - more or less than some threshold.

The procedure of chalcopyrite design included three stages: prediction of new compounds with composition ABX_2, prediction of new chalcopyrites of this composition and estimation of band gap of new chalcopyrites. In order to estimate the reliability of various algorithms the examination recognition was carried out using learning sets. In case of applying system RECOGNITION the collective of recognizing algorithms was used. The following parameters of chemical elements were used for description of chemical compounds:

- electronegativity in the Martynov-Batsanov scale of values $\Delta\chi$, where $\Delta\chi = |2\chi_C - \chi_A - \chi_B|$;
- atomic electrovalent Z_A, Z_B, Z_C (for transition metals, the group number of elements is used as Z);
- mean Born exponent $\bar{n} = \frac{n_A + n_B + 2n_C}{4}$;
- chemical scale χ of Pettifor;
- the proportion: $(I_z / Z)_{AC} = (\frac{I_z}{Z})_A - \left[6 + 0{,}1(\frac{I_Z}{Z})_C\right]$, where I_z - final ionization potential;
- atomic radius.

Data for computer learning had been extracted from database «Bandgap» developed by Baikov Institute [21]. The two classes were considered: **1** – chalcopyrites with $\Delta E>2$ eV and **2** – chalcopyrites with $\Delta E<2$ eV.

Tabl. 1 contains experimental values and results of examination prediction of band gap of known chalcopyrites using separate methods.

Table 1

Prediction of ΔE of known chalcopyrites (calculations using separate methods) (threshold = 2 eV)

Compound	Exp. class	ΔE, eV	EC	LDF	LM	MR	NN	QNN	SVM	SWS	TA	LG	DT	CF	SVR
$CuAlS_2$	1	3,5	1	1	1	1	1	1	1	1	1	1	1	1	1
$CuGaS_2$	1	2,44	2	1	1	1	1	1	1	2	2	1	2	1	1
$CuInS_2$	2	1,5	2	2	1	?	2	2	2	2	2	1	2	2	2
$CuAlSe_2$	1	2,67	2	1	1	1	1	1	1	2	2	1	2	1	1
$CuGaSe_2$	2	1,63	2	1	1	1	1	1	1	2	2	1	2	2	2
$CuInSe_2$	2	0,95	2	2	2	2	2	2	2	2	2	2	2	2	2
$CuAlTe_2$	1	2,06	2	2	2	2	1	1	1	2	2	2	2	1	1
$CuGaTe_2$	2	1,18	2	2	2	2	1	1	2	2	2	2	2	2	2
$CuInTe_2$	2	0,88	2	2	2	2	2	2	2	2	2	2	2	2	2
$AgAlS_2$	1	3,13	2	1	1	1	1	1	1	1	1	1	1	1	1
$AgGaS_2$	1	2,75	2	1	1	1	1	1	1	2	1	1	2	1	1
$AgAlSe_2$	1	2,55	2	1	1	1	1	1	1	2	1	1	2	1	1
$AgGaSe_2$	2	1,65	2	1	2	2	1	1	1	2	2	2	2	2	2
$AgInSe_2$	2	1,24	2	2	2	2	2	2	2	2	2	2	2	2	2
$AgAlTe_2$	2	1,8	2	2	2	2	1	1	2	2	2	2	2	2	2
$AgGaTe_2$	2	1,1	2	2	2	2	1	2	2	2	2	2	2	2	2
$AgInTe_2$	2	0,96	2	2	2	2	2	2	2	2	?	2	2	2	2
$ZnSiP_2$	1	2,07	2	2	1	1	1	2	2	1	1	1	2	1	1
$ZnSiAs_2$	1	2,1	2	2	1	1	1	2	2	1	1	1	2	1	1
$ZnGeN_2$	1	2,9	2	2	1	1	1	1	2	1	1	1	2	1	1
$ZnGeP_2$	1	2,1	2	2	1	1	1	2	2	1	1	1	2	1	1
$ZnGeAs_2$	2	1,16	2	2	2	2	2	2	2	2	2	2	2	2	2
$ZnSnP_2$	2	1,45	2	2	2	2	2	2	2	2	2	2	2	2	2
$ZnSnAs_2$	2	0,74	2	2	2	2	2	2	2	2	2	2	2	2	2
$ZnSnSb_2$	2	0,4	2	2	2	2	2	2	2	2	2	2	2	2	2
$CdSiP_2$	1	2,2	2	2	1	1	1	2	2	1	1	1	2	1	1
$CdGeP_2$	2	1,8	2	2	2	2	1	2	2	1	1	2	2	2	2
$CdGeAs_2$	2	0,53	2	2	2	2	1	2	2	2	2	2	2	2	2
$CdSnP_2$	2	1,16	2	2	2	2	2	2	2	2	2	2	2	2	2
$CdSnAs_2$	2	0,3	2	2	2	2	2	2	2	2	2	2	2	2	2
$AgInS_2$	2	1,9	2	2	2	2	2	2	2	2	2	2	2	2	2
$CdSiAs_2$	2	1,51	2	2	2	2	1	2	2	1	1	2	2	2	2
$CuFeS_2$	2	0,53	1	2	2	1	1	1	2	1	1	1	2	2	2
$CuFeSe_2$	2	0,16	2	2	2	?	1	2	2	2	2	2	2	2	2
$CuFeTe_2$	2	0,1	2	2	2	2	1	2	2	2	2	2	2	2	2
$LiGaTe_2$	1	2,31	2	2	2	1	2	2	2	2	2	2	2	1	1
$LiInTe_2$	2	1,46	2	2	2	2	2	2	2	2	2	2	2	2	2
$AgFeSe_2$	2	0,23	2	2	2	2	1	2	2	2	2	2	2	2	2
$MgSiP_2$	1	2,35	2	1	1	1	1	2	2	1	?	1	2	1	1
$MnGeP_2$	2	0,24	2	2	2	1	1	2	2	1	1	1	2	2	2
$MnGeAs_2$	2	0,6	2	2	2	2	2	2	2	2	2	2	2	2	2

The following methods were used: **EC** - estimates calculation algorithms, **LDF** - Fisher's linear discriminant, **LM** - linear machine, **MR** - algorithm of logical regularities, **NN**

The following methods were used: **EC** - estimates calculation algorithms, **LDF** - Fisher's linear discriminant, **LM** - linear machine, **MR** - algorithm of logical regularities, **NN** - neural networks, **QNN** - *Q*–nearest neighbors, **SVM** - support vector machine, **SWS** - statistically weighted syndromes, **TA** – test algorithm, **LG** – logical regularities of recognized object, **DT** – method of binary decisive trees, **CF**- ConFor, **SVR** - support vector regression. Recognition uses procedure of cross-validation (excepting CF and SVR). The best results were achieved using algorithms of logical regularities and ConFor. The prediction of band gap of new chalcopyrites was carried out using results of algorithms of logical regularities and linear machine on the basis of application of the following collective methods to making a decision [11]: **BM** - Bayesian method, **C&S** - clustering and selection, **DT** - decision templates, **WDM** - Wood's dynamic method, **CS** - convex stabilizer, **CM-MV** - committee method - majority vote, **CM-A** - committee method – average value, and **LC** - logical correction. Previous examination recognition showed that the best results of collective recognition could be achieved using Bayesian method and convex stabilizer strategies (error of predicting equals 0 % at cross-validation). The results of these algorithms were used for making a decision at prediction of band gap of new chalcopyrites (tabl. 2). Thus three new compounds ($ZnAlS_2$, $ZnAlSe_2$ and $BeCN_2$) are promising for opto-electronic applications (tabl. 2).

Table 2

Prediction of ΔE of new chalcopyrites (calculations using collective methods) (threshold = 2 eV)

Compound	Prediction of ΔE	BM	C&S	DT	WDM	CS	CM-MV	CM-A	LC
$ZnAlS_2$	1	1	1	1	?	1	1	1	1
$ZnAlSe_2$	1	1	1	1	1	1	1	1	1
$ZnAlTe_2$	2	2	2	2	?	2	2	2	2
$AgFeS_2$	2	2	2	2	2	2	2	2	2
$AgFeTe_2$	2	2	2	2	2	2	2	2	2
$ZnGaTe_2$	2	2	2	2	?	2	2	2	2
$CdGaTe_2$	2	2	2	2	?	2	2	2	2
$HgGaTe_2$	2	2	2	2	?	2	2	2	2
$BeCN_2$	1	1	1	1	1	1	1	1	1

Designation: ? – vague result

Conclusions

The new approach to computer-aided design of inorganic substances, proposed by us, allows an expansion of capabilities of traditional CAD-systems. In this case the information of DBs on inorganic material and substance properties is used not only as handbook for selection of known materials but as a basis for a search for regularities and predicting new, not yet synthesized, substances with predefined properties. Thus new substances are designed from chemical elements which are included into their composition. Proposed approach allows overcoming of material limitation at traditional design of devices, machines, etc.

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СОДЕРЖАНИЕ

СХЕМОТЕХНИЧЕСКОЕ, ТОПОЛОГИЧЕСКОЕ И ФИЗИЧЕСКОЕ ПРОЕКТИРОВАНИЕ