Design of Inorganic Compounds with the Use of Precedent-Based Pattern Recognition Methods

Yu. I. Zhuravlev[a], N. N. Kiselyova[b], V. V. Ryazanov[a], O. V. Sen'ko[a], and A. A. Dokukin[a]

[a] *Dorodnicyn Computing Center, Russian Academy of Sciences, ul. Vavilova 40, Moscow, 119333 Russia*
[b] *Baikov Institute of Metallurgy and Materials Science, Russian Academy of Sciences, Leninskii pr. 49, Moscow, 119991 Russia*
e-mail: zhuravlev@ccas.ru, kis@imet.ac.ru, rvvccas@mail.ru

Abstract—The possibility of searching for classification regularities in large arrays of chemical information with the use precedent-based recognition methods is discussed. The results of application of these regularities to the computer-assisted design of inorganic compounds promising for the search for new materials for electronics are presented.

Keywords: precedent-based recognition, prediction of properties, computer-assisted design of inorganic compounds, magnetic materials.

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INTRODUCTION

Pattern recognition methods are widely used in natural sciences, especially in those in which it is difficult to develop accurate mathematical models: chemistry and materials science [1–4], biology [5], geology [6, 7], medicine [8, 9], etc. At the modern level of development of computational mathematics, even complex algebraic constructions do not guarantee satisfactory computational results for the objects and phenomena studied in the above-mentioned fields of science. However, in each field of science, various classification schemes have been developed and are used, since obtaining any scientific knowledge requires two initial stages: data acquisition and data classification. In most empirical sciences, classification schemes play the role of exact mathematical regularities. The development of classification rules is a complicated and laborious process that requires high qualifications of specialists. These rules are often named after their authors, for example, the Darken–Gurry rule for predicting mutual solubility of metals [10], the Matthias criterion for predicting new superconductors with the A15-type of crystal structure [11], etc. The application of pattern recognition methods and appropriate software systems allows one to facilitate and speed up the development of classification rules. The tasks of a specialist in a specific subject field when implementing this process are reduced to the statement of a problem, choice of objects and phenomena for computer-assisted analysis, choice of the feature description, interpretation of the results, and application of the classification rules to prediction.

The present paper is devoted to the use of precedent-based computer training methods for searching for classification rules for inorganic substances and the application of these rules to predicting new compounds and evaluating their properties.

1. STATEMENT OF THE PROBLEM

Suppose that every inorganic substance is described by a vector $\mathbf{x} = (x_1^{(1)}, x_2^{(1)}, ..., x_M^{(1)}, x_1^{(2)}, x_2^{(2)}, ..., x_M^{(2)}, ..., x_1^{(L)}, x_2^{(L)}, ..., x_M^{(L)})$, where L is the number of chemical elements that form a compound and M is the number of parameters of the chemical elements. Each substance is also characterized by a membership parameter in a class: $a(x) \in \{1, 2, ..., K\}$, where K is the number of classes. The training sample consists of N objects: $\mathbf{S} = \{\mathbf{x}_i, i = 1, ..., N\}$. We denote a subset of objects of the training sample from class $a_j, j = 1, 2, ..., K$, by $\mathbf{S}_{aj} = \{x: a(x) = a_j\}$. The aim of training is to construct a classification rule that distinguishes not only between objects of different classes in the training sample but also between all the other combinations of chemical elements. Thus, we deal with the classical statement of a precedent-based pattern recognition problem. The specific feature of the subject field manifests itself only in the formation of the feature description, which has a composite structure: the set of parameters of chemical elements (the components of

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an inorganic substance) is repeated as many times as there are elements included into the compound.

As a rule, the following classification problems are solved most successfully in inorganic chemistry:

—classification of combinations of chemical elements into systems with and without the formation of compounds (eutectic systems, systems with solid solutions, heterogeneous mixtures, etc.) in the entire range of concentrations of the components and in a given range of temperatures and pressures;

—classification of combinations of chemical elements into systems with and without the formation of compounds of certain composition in a given range of temperatures and pressures;

—classification of inorganic compounds of given composition according to the type of crystal structure at certain temperatures and pressures;

—classification of inorganic compounds of a given composition into compounds whose functional properties are above or below a given threshold value under certain external conditions (for example, melting temperature, band gap energy, etc.).

2. INFORMATION–ANALYTICAL SYSTEM FOR DESIGNING INORGANIC COMPOUNDS

For computer-assisted analysis (computer training), we use a specially developed information–analytical system (IAS) that includes databases (DBs) on the properties of inorganic substances and materials and a software complex for pattern recognition [12–14]. Today, the IAS includes DBs developed at the Baikov Institute of Metallurgy and Materials Science, Russian Academy of Sciences [3, 12–14]; these are "Phases," a DB on the properties of inorganic compounds; "Elements," a DB on the properties of chemical elements; "Diagram," a DB on the phase diagrams of semiconductor systems; "Crystal," a DB on the properties of acousto-optical, electro-optical, and nonlinear-optical substances; and "Bandgap," a DB on the band gap of inorganic substances. The subsystem for data analysis, searching for classification regularities, and predicting incorporates software programs of the RECOGNITION system, which was developed at the Computing Centre, Russian Academy of Sciences [15]; these programs are based on linear machine methods, Fischer's linear discriminant, *k*-nearest neighbors, support vector machine, neural network algorithms, estimate calculation algorithms, algorithms for voting by irreducible tests, for voting by systems of logical regularities, statistical weighted voting, etc. The IAS also includes ConFor software for training a computer for concept formation, which was developed at the Institute of Cybernetics, National Academy of Sciences of Ukraine [16], and is based on the organization of data in computer memory in the form of growing pyramidal networks. The subsystem for data analysis also uses various collective decision making methods: the Bayes method; clustering and selection, decision templates, logical correction, and convex stabilizer; the Woods dynamic method; committee methods; etc. [15]. The IAS is designed for the automation of storing and updating information, preparation of data for analysis, search for classification rules and prediction, and visualization and representation of the results of data analysis.

3. EXPERIMENTAL RESULTS ON THE COMPUTER-ASSISTED DESIGN OF INORGANIC COMPOUNDS

The problem of designing new inorganic compounds can be formulated as follows [3, 14]: Find a set of chemical elements and their proportion (i.e., the qualitative and quantitative composition) for designing (under given external conditions) a crystal or molecular structure of a compound that would provide necessary functional properties. The source information for predicting new compounds is solely the data on the properties of the chemical elements.

The IAS has been intensively used for the design of new inorganic compounds that are promising for searching for new magnetic, semiconductor, acousto-optical, electro-optical, nonlinear-optical, and other materials for electronics [12–14].

3.1. Computer-Assisted Design of AB_2X_4 (X = S, Se, or Te) Compounds That Are Promising in the Search for New Semiconductors

Most of the AB_2X_4 compounds are semiconductors. AB_2X_4-type chalcogenide spinels (X = S, Se, or Te) are of interest in relation to the search for new magnetic semiconductors with a composition similar to that of $CdCr_2S_4$, $CdCr_2Se_4$, $HgCr_2Se_4$, $ZnCr_2Se_4$, $CuCr_2S_4$, $FeCr_2S_4$, etc., which were discovered in the 1960s [17–20]. Chalcogenide spinels can also be used in magnetic-field controlled narrow-band light sources [17–19]. It is promising to use chalcogenide spinels in integrated circuits in which one region is used as an active semiconductor device and another, as a magnetic microwave device, as well as in devices where the interaction between electric, magnetic, and optical properties plays a significant role [17]. Interest in chalcogenide spinels is also stimulated by the weak superconductivity that has been observed in some compounds of this type [21]: in $CuRh_2S_4$ (the critical temperature $T_c = 4.8$ K), $CuRh_2Se_4$ ($T_c = 3.49$ K), and CuV_2S_4 ($T_c = 4.45$ K). Chalcogenide spinels are considered as promising thermoelectric materials [22].

First, the IAS has allowed us to predict the possibility of formation of AB_2X_4 compounds (A and B are various elements; X = S, Se, or Te). For training the system, we used 835 examples of formation of compounds (class 1) and 154 examples of the absence of compounds with this composition (class 2) under

Table 1. Properties of elements used for the description of AB_2X_4 compounds (prediction of formation of compounds)

No.	Property	No.	Property
1	(Zunger) pseudopotential radius	13	First ionization energy
2	Melting point	14	Second ionization energy
3	Covalent radius	15	Third ionization energy
4	Quantum number	16	Miedema chemical potential (only for elements A and B)
5	(Schubert) distance to core electrons	17	Group number (only for elements A and B)
6	(Schubert) distance to valence electrons	18	(Mendeleev–Pettifor) regular number
7	(Bokii and Belov) ionic radius	19	Debye temperature (only for elements A and B)
8	Boiling point	20	Molar heat capacity
9	Enthalpy of vaporization	21	Solid state entropy
10	Enthalpy of melting	22	Thermal conductivity
11	(Martynov and Batsanov) electronegativity	23	Number of valence electrons (only for elements A and B)
12	Enthalpy of atomization		

standard conditions. Information was retrieved from the DB "Phases" [3, 13].

In the computer memory, chemical systems were represented as a set of properties of the chemical elements A, B, and X (Table 1). Information on the properties of the chemical elements was extracted from the DB "Elements" [13].

After the analysis of the data, which involved several computer training algorithms, we carried out an examination recognition with cross validation on the training sample. The quality (accuracy) of the algorithm was assessed as the percentage of correctly recognized objects. By the results of the examination recognition, we chose the best computer training algorithms for further use in collective decision making methods, namely, Fischer's linear discriminant (with 87.6% of correctly recognized objects), the neural-network algorithm (86.7%), and the *k*-nearest neighbors algorithm (80%).

The best algorithm for collective decision making when solving this problem and like questions was chosen on the basis of recognition of 100 objects chosen randomly by a uniform distribution. These objects were eliminated from the training sample both during the training process and during the tuning of collective decision making algorithms. By the results of recognition of 100 objects, we evaluated the accuracy of collective decision making. From the set of constructed recognition algorithms and algorithms for collective decision making, we chose a subset of the most accurate algorithms.

At the final stage, the processes of training of the chosen algorithms were initiated again on the original training sample. As a result, the four designed prediction models included the following algorithms: Fisher's linear discriminant, neural networks, *k*-nearest neighbors, algorithms for making collective decisions by the Bayes method, logical correction, decision templates, and clustering and selection. When predicting new compounds, these models were applied independently. The results of prediction by these four methods were juxtaposed. The decision on the formation of an AB_2X_4 compound was made when the predictions were not contradictory.

Next, we predicted the type of the crystal structure of AB_2X_4 compounds (X = S, Se, or Te) at room temperature and atmospheric pressure. The feature description included the parameters of the chemical elements, which are listed in Table 1. In view of the importance of the atomic size of the elements in the formation of crystal structures, we added one more property: $(R_{covA} - R_{covB})/R_{covX}$, where R_{cov} is the covalent radius of an appropriate element. First, we carried out a multiclass prediction, where we simultaneously considered 17 classes: **1**, an AB_2X_4 compound with the spinel structure (75 examples); **2**, compounds with the olivine structure (18 examples); **3**, compounds with the structure of $MnEr_2Se_4$ (24 examples); **4**, compounds with the structure of $CdAl_2S_4$ (21 examples); **5**, compounds with the structure of $PbGa_2Se_4$ (37 examples); **6**, compounds with the structure of β-K_2SO_4 (14 examples); **7**, compounds with the structure of $CaFe_2O_4$ (73 examples); **8**, compounds with the structure of ThP_4 (92 examples); **9**, compounds with the structure of $NiCr_2S_4$ (38 examples); **10**, compounds with the structure of $CaHo_2Se_4$ (13 examples); **11**, compounds with the structure of $PbBi_2S_4$ (5 examples); **12**, compounds with the structure of $GeSr_2S_4$ (7 examples); **13**, compounds with the structure of

TlSe (3 examples); **14**, compounds with the structure of $PbCr_2S_4$ (8 examples); **15**, compounds with the sphalerite structure (4 examples); **16**, compounds with a structure different from those listed above (23 examples); and **17**, an AB_2X_4 compound is not formed under normal conditions (154 examples). Then, to increase the reliability of prediction, for classes **1**–**5** and **7**–**10**, we solved problems in which all chemical systems were classified into three groups: (*1*) the goal group (for example, compounds with the spinel structure), (*2*) all the compounds with crystal structures different from the structures of the goal group, and (*3*) nonformation of AB_2X_4 compounds.

When making collective decisions, we used methods that gave the best results in the test recognition (in most cases, these were linear machine methods, voting by logical regularities, *k*-nearest neighbors, statistical weighted voting, and two-dimensional linear separators). The application of collective methods (the Bayes method, clustering and selection, decision templates, logical correction, and committee methods) has allowed us to increase the reliability of prediction.

As a result, for each of the three compositions AB_2X_4 (X = S, Se, and Te), we obtained eleven tables of predictions (a table of prediction of the possibility of formation of a compound, a table of multiclass prediction, and nine tables of predictions for classes **1**–**5** and **7**–**10**, in which all chemical systems were classified into three groups). Next, we compared the predictions from these eleven tables and made a decision on the formation of a given compound and its crystal structure provided that the predictions were not contradictory.

Table 2 shows a part of the predictions of the crystal structure type for AB_2Se_4 compounds. We used the following notations: **1**, prediction of the spinel-type structure; **2**, prediction of the olivine-type structure; **4**, prediction of the $CdAl_2S_4$-type structure; **5**, prediction of the $PbGa_2Se_4$-type structure; **7**, prediction of the $CaFe_2O_4$-type structure; **8**, prediction of the Th_3P_4-type structure; **9**, prediction of the $NiCr_2S_4$-type structure; **10**, prediction of the $CaHo_2Se_4$-type structure; **11**, prediction of the $PbBi_2S_4$-type structure; **12**, prediction of the $GeSr_2S_4$-type structure; **14**, prediction of the $PbCr_2S_4$-type structure; **15**, prediction of the sphalerite-type structure under normal conditions; **16**, prediction of a crystal structure different from those listed above; and **17**, prediction of the nonformation of AB_2Se_4 compounds under normal conditions; the sign # marks objects that were used during computer training; the empty cells refer to the case when predictions made with the use of different collective decision making methods do not coincide, or when an uncertain prediction is made.

3.2. Computer-Assisted Design of Heusler Phases with Composition ABX_2 (X = Mg, Al, Fe, Co, Ni, Cu, Ru, Rh, Pd, Ag, Ir, Pt, or Au) That are Promising for Searching for Magnetic Materials

ABX_2 compounds with a Heusler-phase-type crystal structure have long attracted the attention of researchers as promising magnetic materials [23–29]. In recent years, special interest in these phases has been stimulated by the development of high-capacity magnetic memory devices, including spintronic devices [30–34].

For computer training, we used information on 278 known Heusler phases of ABX_2 composition, 70 compounds with the structure of $MgCuAl_2$, 38 compounds with the structure of $YSiPd_2$, 20 compounds with the structure of NaTl, 11 compounds with the structure of $PrGaCo_2$, 10 compounds with the structure of $YSiRh_2$, 16 compounds with the structure different from those listed above, and 486 examples of nonformation of ABX_2 compounds (A and B are various elements, and X is Mg, Al, Fe, Co, Ni, Cu, Ru, Rh, Pd, Ag, Ir, Pt, or Au). Information was extracted from the DB "Phases" on the properties of inorganic compounds [3, 12–14].

Information on metal systems was represented in the computer memory as a set of properties of the chemical elements A, B, and X, which included the following parameters: the (Zunger) pseudopotential radius; enthalpy of vaporization; melting point; boiling point; Debye temperature; the first three ionization potentials; (Schubert) distances to core and valence electrons; (Mendeleev–Pettifor) regular number; (Pauling) electronegativity, Miedema chemical potential; quantum number; heat conductivity; group number in the Periodic System; molar heat capacity; enthalpies of melting, vaporization, and atomization; solid state entropy; atomic weight; density; linear thermal expansion coefficient; (Weber) metallic radius; etc. (108 parameters for each substance in total). The data on the properties of elements were taken from the DB "Elements" [13].

The prediction procedure for the type of the crystal structure of intermetallic compounds included three tasks:

(1) Prediction of A–B–X chemical systems (A and B are various elements, and X is Mg, Al, Fe, Co, Ni, Cu, Ru, Rh, Pd, Ag, Ir, Pt, or Au) with the formation and nonformation of ABX_2 compounds.

(2) Multiclass prediction of the type of crystal structure (nine classes): **1**, Heusler phases; **2**, compounds with the structure of NaTl; **3**, compounds with the structure of $YSiRh_2$; **4**, compounds with the structure of $MgCuAl_2$; **5**, compounds with the structure of $GdSnPt_2$; **6**, compounds with the structure of $YSiPd_2$; **7**, compounds with the structure of $PrGaCo_2$; **8**, compounds with the structure different from those listed above; and **9**, the nonformation of ABX_2 compounds.

Table 2. Predictions of the type of crystal structure of AB_2Se_4 compounds under normal conditions

A B	Be	Mg	Ca	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	Sr	Pd	Ag	Cd	Sn	Ba
B	16		5								17	17		17	5	17	17	#17	17	
Al		#16	#5				4		4			#4	17		#5			#4		#16
P	16	16	5												5		17			14
Se	2	#1					#1					1		2	7			1		7
Ti	9				#9	9	#9	#9	#9	#9	1	1				9	1	1		7
V	9			9		#9	#9	#9	#9	#9	1	1			#14	9	1	1		
Cr		1		#9	9		9	9	9	#9	#1	#1		#17	14		1	#1	14	14
Mn	7	1		9	9	9		9	9	9	#1	#1			2	9	1	1	2	2
Fe		1		#9	#9	9	9		9	9	1	1		2		9	1	1		16
Co		1		9	9	9		9		9	1	1					1	1		16
Ni		1		9	9						1	1					1	1	17	16
Ga		16	#5				#4				#15	#4		#17	#5	17	15	#4	#17	#5
As			11								17	#17	#17	#17	16		#17	#17		11
Y	2	#1	#10		9	9		9	9	9		1	10	2	#7			#1		#7
Mo		1		9	9	9	9	9	9	9	1	1					1	1	14	
Rh	16	1		9	9	#9			#9	#9	#1	1		15			1	1		
In	17	#16	#16				#16					#16	17	#17	16	17	17	4	#17	16
Sb	16	16	16								17		17		16		17			
La	12	8	8			#8	12		12	12			8	12	8	16		#8	8	
Ce	12	8	8			#8	12	12	12	12			12	12	8	12		8		
Pr	12	8	8			#8					17			12	8	16	17	8	8	
Nd	12	8	8			#8	16				#17			12	8	16	17	#8	#16	7
Pm	2	8	8			8					17			2		16	17	8	2	7
Sm	12	8	8	16		#8					17			12	8	16	17	8		#7
Eu	12	8		12		#8	12	12	12	12				12	8	12		8	12	7
Gd		8									#17			12	8			#8		#7
Tb		16					10							2	#7			#8		7
Dy		1	#10									1		2	#7			#1		#7
Ho		#1	#10									1		2	#7			#1		7
Er		#1	#10									1		2	#7			#1		7
Tm	2	#1	10						2			1		2	#7			#1		7
Yb	12	#1	#10	12				12	12	12		1		#12	#7	12		#1		#7
Lu	2	#1	#10	10					2			1		2	#7			#1		#7
Ir		1	11								1	1					1	1		
Au		1	17	17	17	17	17			17	17		17	17		17			#17	
Tl		16	10								17		17		16	17	#17		#17	
Bi		16	16								17	#17	17	16	#16	17	17			
Th	12	8		9	9	9	9	9	9	9				12	8		17			
Pa	12	8		9	9	9	9	9	9	9				12	8		17			
U	16	16			9		9	9	9					2	8	16	17		2	
Np	12				9		9	9	9			1		12	8	16			2	
Pu	12	8		9	9		9	9	9	9		16		12	8	16		8		

Table 3. Predictions of the type of crystal structure of $ABCo_2$ compounds

A / B	Li	Be	Mg	Al	Si	Sc	Ti	V	Cr	Mn	Fe	Ni	Cu	Zn	Ga	Ge	Y	Zr	Nb	Ru	Pd	Ag	In	Sn	Sb	La	Ce	Pr	Nd	Pm	Sm	Gd	Tb	Hf
Be	1																																
Si	1	#1																															
Sc				#1	1																												
Ti			1	#1	#1	1																											
V			1	#1	#1	1																											
Cr				#1		1																											
Mn	1				#1	1																											
Fe		6	6	6	6	6	6	6	6	#6																							
Ni		6	6	6	6		6	6	6	6	#6																						
Cu	5	6	6		#6	5	6	6	6	6	#6	6																					
Zn		6	6			5		6	6	6	6	6	6																				
Ga						#1	#1	#1		#1			6	6																			
Ge	#1	#1				#1	#1	1		#1	6	6	6	#1	6			1	1	6													
Zr				#1			1				6	#6	6		1	1																	
Nb				#1								6	6		1	1				6	6												
Ru		6	6	6	6		6	6	6	6	6	6	6	6	6	6		6	6		6	6	6	6									
Pd		6			6		6	6	6	#6	#6	#6	#6	6	6	6		6	6	6		#6	6	6									
Ag					6						6	6	6	6						6	#6		6	6									
In					6						6	6	6	6						6	6	6		6									
Sn					6						6	6	6	6						6	6	6	6	6									
Sb					6						6	6	6	6						6	6	6	6	6									
La					6						6	6	6	6						6	6	6	6	6									
Ce					6						6	6	6	6						6	6	6	6	6									
Pr					6						6	6	6	6						6	6	6	6	6									
Nd					6						6	6	6	6						6	6	6	6	6									
Pm					6						6	6	6	6						6	6	6	6	6									
Sm					6						6	6	6	6						6	6	6	6	6									
Eu					6						6	6	6	6						6	6	6	6	6									
Gd					6						6	6	6	6						6	6	6	6	6									
Tb					6						6	6	6	6						6	6	6	6	6									
Dy					6						6	6	6	6						6	6	6	6	6									
Ho					6						6	6	6	6						6	6	6	6	6									
Er					6						6	6	6	6						6	6	6	6	6									
Tm					6						6	6	6	6						6	6	6	6	6									
Yb					6						6	6	6	6						6	6	6	6	6									
Lu					6						6	6	6	6						6	6	6	6	6									
Hf				#1							6	6	6	6	1	1		6	6	6	6	6	6	#1		4							6
Ta				#1							6	6	6	6	#1	1		6	6	6	6	6	6	1		4							1
Pt		6	6	6		6	6	6	6	6	6	6	6	6	6	6		6	6	6	6	6	6	6							4		
Tl											6	6	6	6						6	6	6	6	6									
Pb											6	6	6	6						6	6	6	6	6									
Bi						6	1		6	1															6								
Th				4			1	1		1			2	2									4	4									
U													2	2																			

(3) For classes **1**–**7**, successive division of systems into three classes, for example, class **1**, the Heusler phases; class **2**, compounds with the structure different from the Heusler phases; and class **3**, the absence of ABX_2 compounds in the A–B–X system.

The best algorithms according to the results of examination recognition with cross validation (mostly, these were linear machine methods, formation of logical regularities, *k*-nearest neighbors, and ConFor) were used for collective decision making. From among these algorithms, we chose the most efficient methods (most frequently, this was the complex committee method—averaging), which were used for predicting new compounds. Note that the application of collective algorithms has allowed us to substantially increase the reliability of prediction.

As a result, for each of 13 ABX_2 compounds (A and B are various elements, and X is Mg, Al, Fe, Co, Ni, Cu, Ru, Rh, Pd, Ag, Ir, Pt, or Au), we obtained nine tables of predictions (a table of prediction of the possibility of formation of a compound, a table of multiclass prediction, and seven tables of predictions for classes **1**–**7**, in which all metal systems are classified into three groups). Next, we compared the predictions from these nine tables and made a decision on the existence of a given compound and on the type of its crystal structure provided that the predictions were not contradictory. Table 3 shows a part of predictions obtained in this way for new Heusler phases of $ABCo_2$ composition. We used the following notations: **1**, a compound with the crystal structure of Heusler phases; **2**, a compound with the structure of $YSiRh_2$; **4**, a compound with the structure of $PrGaCo_2$; **5**, a compound with the structure different from those listed above; and **6**, the nonformation of a $ABCo_2$ compound. The sign # marks systems information that was used for computer training. The empty cells refer to the cases when predictions obtained at different stages do not coincide.

4. CONCLUSIONS

The application of precedence-based pattern recognition methods to the computer-assisted design of inorganic compounds allows one to find complex classification regularities that make it possible to predict the membership of new chemical systems in one class of substances or another on the basis of knowledge of the well-known properties of the components of these systems—chemical elements. Computer-assisted design allows one to substantially reduce the number of complex and expensive experiments in the search for inorganic compounds with predefined properties, replacing them by computation. The experimental verification of the results of computer-assisted design shows that the average accuracy of predicting is higher than 80% [1–3, 14].

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Yurii Ivanovich Zhuravlev. Born 1935. Graduated from the Moscow State University in 1957. Received doctoral degree in 1965, Professor since 1967, and Academician of the Russian Academy of Sciences since 1992. Currently Deputy Director of the Dorodnicyn Computing Center, Russian Academy of Sciences, Chair at the Mathematics Department of the Russian Academy of Sciences, and Head of Chair at Moscow State University. Editor-in-Chief of *Pattern Recognition and Image Analysis.* Foreign member of the Spanish Royal Academy of Sciences, the National Academy of Sciences of Ukraine, and the European Academy of Sciences. Winner of the Lenin and Lomonosov Prizes. Scientific interests: mathematical logic; control systems theory; mathematical theory of pattern recognition, image analysis, and forecasting; operations research; and artificial intelligence.

Nadezhda Nikolaevna Kiselyova. Born 1949. Graduated from the Department of Chemistry, Moscow State University, in 1971 and postgraduate course at the same department in 1974. Received candidates degree in 1975 and doctoral degree in 2004. Currently is Head of Laboratory of Semiconductor Materials at the Baikov Institute of Metallurgy and Materials Science, Russian Academy of Sciences. Scientific interests: computer-assisted design of inorganic compounds, databases on the properties of inorganic substances and materials, and electronic materials. Author of more than 130 papers and 2 monographs.

Vladimir Vasil'evich Ryazanov. Born 1950. Graduated from the Moscow Institute of Physics and Technology in 1973. Received candidates degree in 1979 and doctoral degree in 1994. Academician of the Russian Academy of Natural Sciences, Professor. Since 1976 has been with the Dorodnicyn Computing Center, Russian Academy of Sciences. Currently is Head of the Department of Mathematical Problems of Recognition and Methods of Combinatorial Analysis. Scientific interests: recognition theory, cluster analysis, data analysis, optimization of recognition models, and applied systems of analysis and prediction.

Oleg Valentinovich Sen'ko. Born in 1957 in Salavat, Bashkortostan. Graduated from the Moscow Institute of Physics and Technology in 1981. Received candidates degree in 1990 and doctoral degree in 2007. Currently is a senior researcher at the Dorodnicyn Computing Center, Russian Academy of Sciences. Scientific interests: data mining, mathematical models of pattern recognition, classification and forecasting, practical applications in medicine and other fields.

Aleksandr Aleksandrovich Dokukin. Born 1980. Graduated with honors from the Department of Computational Mathematics and Cybernetics, Moscow State University, in 2002. Received candidates degree in 2005. Currently is a researcher at the Dorodnicyn Computing Centre, Russian Academy of Sciences. Author of more than 30 papers.