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Prediction of the Crystal Structure Types of Equiatomic Ternary Silicides and Germanides

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Abstract—New unsynthesized equiatomic *ABX* (*A* and *B* are various metals; *X* = Si or Ge) compounds are predicted, and their types of crystal structure are forecasted under standard conditions. Only the data on the properties of the elements—components of compounds are used for their prediction. The calculations are performed using a special-purpose software package of computer analysis of information intended for searching for regularities in databases on the properties of inorganic compounds, and this package is based on the methods of precedent pattern recognition. Computer analysis of the data on the well-known compounds shows that the functions that are most important for the classification of systems in the sign of formation or absence of equiatomic compounds are $M(A) \times M(B)$ and $I(A) \times I(X)$, where *M* is the Mendeleev–Pettifor number of element *A* or *B* and *I* is the thermal conductivity of element *A* or *X*. The parameters that most strongly separate compounds for crystal chemical classification are functions $T(A) + T(B)$ (where *T* is the melting temperature of element *A* or *B*), $I(A)$, $M(A) \times M(B)$, and $I(A) \times I(X)$.

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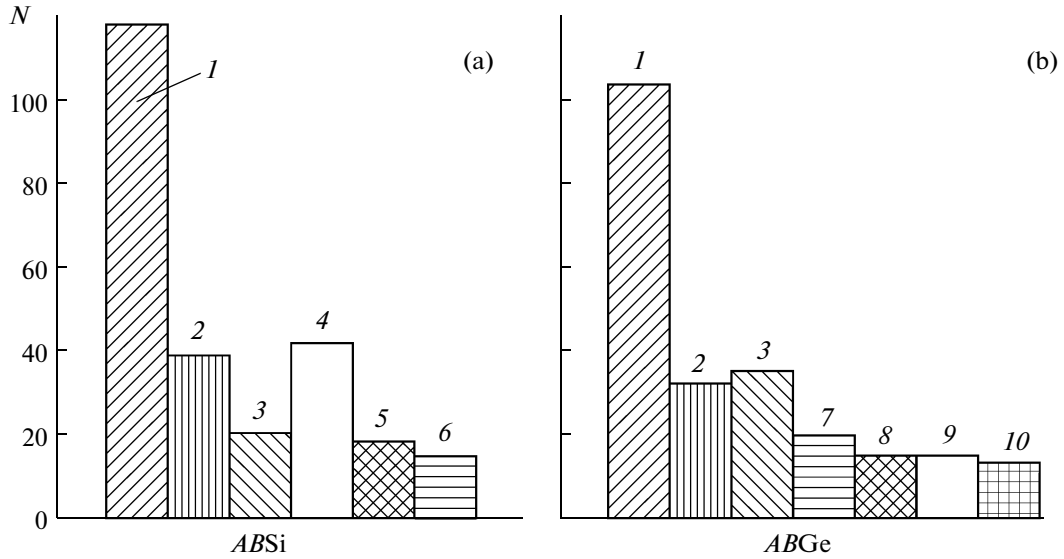
INTRODUCTION

In recent years, *ABX* (*A* and *B* are various metals; *X* = Si or Ge) compounds have been extensively studied due to searching for new magnetic materials [1–6]. More than seven hundred compounds of this composition have been synthesized to date, and most of them have structure types TiNiSi, ZrNiAl, or PbFCl (figure).

THEORETICAL ANALYSIS

Based on an analysis of the experimental data on the well-known ternary equiatomic silicides and germanides, researchers [7–17] tried to find the regularities that can be used to predict the formation and type of crystal structure of unknown compounds using only data on the component parameters. To predict the types



Distribution of studied *ABX* compounds (*N* is the number of compounds) over the types of crystal structure: (*1*) TiNiSi, (*2*) PbFCl, (*3*) ZrNiAl, (*4*) AlB_2, (*5*) α-$ThSi_2$, (*6*) YPtAs, (*7*) LiGaGe, (*8*) LaPtSi, (*9*) CeScSi, and (*10*) TiFeSi.

of crystal structure of rare-earth metal (R) ARX compounds, the authors of [7] proposed to use the following element parameters: the size parameter $f(r) = r_R/(r_A + r_X)$, where r_R, r_A, and r_X are the metallic radii of R, A, and X, respectively [18]; the electrochemical parameter $f(\Phi^*) = \Phi_A^* + \Phi_X^* - \Phi_R^*$, where Φ^* is the electronegativity on the Miedema scale [19]; the element period number in the periodic system; and the valence electron concentration, which is the ratio of the total number of valence electrons to the number of atoms in an intermetallic lattice. However, when trying to construct the projection of the points corresponding to the well-known equiatomic silicides and germanides onto the plane with the coordinates proposed in [7] (i.e., parameter $r_R/(r_A + r_X)$ and the valence electron concentration), we failed to correctly separate the regions of compounds with different types of crystal structures.

The authors of [8] studied the dependences of the type of crystal structure of rare-earth metal ARX silicides, germanides, and gallides on the group number and the period number of elements A and X in the periodic system and the atomic number and the ionic radius of R metals. Based on experimental information, the authors of [9–11] made a conclusion regarding the key role of the atomic size for predicting the type of crystal structure of rare-earth metal R equiatomic compounds. According to [12], the most important parameter for solving this problem is the ratio of the atomic radius of metals R to atomic radius of A. In these works, researchers only considered rare-earth metal R compounds. The authors of [13] tried to predict the type of crystal structure of transition metal A and B equiatomic compounds and stated that the type of crystal structure depends on the Miedema electronegativity [19] and the electron density of a pure metal. The necessity of taking into account the sum and difference of the metallic radii of elements A and B for predicting the type of crystal structure of the equiatomic compounds where X = Si, Ge, Sn, or Pb was noted in [14]. The dependence of the type of crystal structure on the valence electron concentration was studied in [15]. Apart from this parameter, the authors of [16] suggested to use the element X period number and the size parameter $f(r) = r_A/(r_B + r_X)$ to predict the type of crystal structure of ABX (X = Si, Ge, Sn, Pb) compounds.

Thus, as a result of an analysis of the experimental data on the equiatomic compounds studied in [7–16], the following main component parameters that determine the type of crystal structure were established: the size of atoms, the atom position in the periodic system, the valence electron concentration, the electron density at the edge of the Wigner–Seitz cell [19], and the electronegativity of a chemical element. Naturally, taking into account these parameters is a necessary condition for searching for the regularities of formation of various crystalline intermetallic phases. However, the question arises as to whether these properties are sufficient to predict unknown compounds. In [17], we proposed another method, which implies the use of the wide spectrum of the well-known properties of elements to predict new equiatomic compounds. One of the purposes of this work is to compare these two prediction methods, namely, the use of only the most important element parameters or the use of all well-known properties of elements. Based on this comparison, we developed a technique to predict new ternary equiatomic silicides and germanides and predicted new unknown phases.

EXPERIMENTAL COMPUTER TECHNIQUE

The solution of the problem included the following stages:

(i) the selection of examples of equiatomic compounds for computer analysis;

(ii) the selection of the properties of elements to form a classifying rule;

(iii) the selection of the properties of elements that are most important for classification and the selection of the simplest algebraic function of these properties using the program of searching for classifying parameters [20];

(iv) the choice of the algorithms of computer data analysis, which are based on precedent pattern recognition methods and are intended for searching for classifying criteria, and computer training;

(v) the search for classifying criteria using computer training methods for chosen examples of the well-known substances and the prediction of the formation and the type of crystal structure of new ternary equiatomic silicides and germanides under standard conditions (298 K, 0.1 MPa) using the found criteria.

We now consider the work done at each stage.

Selection of the Examples of Compounds for Computer Analysis

The initial information for computer analysis consists of a matrix each line in which corresponds to a well-known substance and represents a set of the values of properties of the components, i.e., chemical elements A, B, and X.

Each line also corresponds to the value of a target parameter (e.g., the designation of the type of crystal structure). This matrix is called a learning sample, and its representativeness and reliability substantially determine the accuracy of the subsequent prediction. As a rule, the selection of the examples of inorganic substances for computer analysis is performed by qualified chemists using the databases on the properties of inorganic substances and materials (including the database of the Baikov Institute of Metallurgy and Materials Science [21]), which contain information on several tens of thousands of substances and are accessible for authorized users on the Internet (http://imet-db.ru).

Selection of the Properties of Elements to Form a Classifying Rule

The selection of the properties of components that are important for the classification of inorganic compounds is the most difficult problem that affects the prediction quality. As a rule, the properties of chemical elements are taken from the database "Elements" developed by us (http://phases.imet-db.ru/elements) [21]. In this work, we use the physicochemical concepts of the nature of the phases under study and include the following parameters of elements A, B, and X in the initial set of the properties of elements: the pseudopotential radii [22], the melting and boiling temperatures, the first three ionization potentials, the distances from core and valence electrons (according to Schubert), the group number in the periodic system, the quantum number, the element numbers (after Mendeleev–Pettifor) [23, 24], the Pauling electronegativity, the Miedema electronegativity, the Miedema chemical potential, the values of Miedema function $n_{WS}^{1/3}$ (where n_{WS} is the electron density at the edge of the Wigner–Seitz cell [19]), the thermal conductivity, the molar heat capacity, the enthalpies of vaporization and atomization, the entropy for a solid state, the metallic radii [18], the number of valence electrons, and so on (in total, 92 parameters for each chemical system).

Selection of the Properties of Elements That Are the Most Important for the Classification

In this work, we solve the following three successive classification problems:

Problem 1 consists in searching for a criterion to divide A–B–X systems into systems with the formation of equiatomic compounds and systems in which such compounds do not form under standard conditions.

Problem 2 consists in searching for a criterion to divide A–B–X systems into the following five classes: (1) systems with the formation of equiatomic compounds with a TiNiSi-type crystal structure (space group $Pnma$, $Z = 4$), (2) systems with ABX compounds with a ZrNiAl-type crystal structure (space group $P\bar{6}\,2m$, $Z = 3$), (3) systems with ABX compounds with a PbFCl-type crystal structure (space group $P4/nmm$, $Z = 2$), (4) systems with equiatomic compounds with a structure that differs from those given above under standard conditions, and (5) A–B–X systems without the formation of equiatomic compounds.

Problem 3 consists in searching for a criterion to successively divide systems into three classes (e.g., target class 1, compounds with a TiNiSi-type crystal structure; class 2, compounds with a structure other than TiNiSi; and class 3, the absence of equiatomic compounds in an A–B–X system).

To find the set of properties of elements and the simplest algebraic functions of these properties that are most important for solving these problems, we used the computer program included in the information-analytical system (IAS) developed at the Institute of Metallurgy and Materials Science for computer-assisted design of inorganic compounds [25]. This program is based on the minimization of generalized error functionals for convex correcting procedures with respect to ensembles of predictors constructed on the basis of individual attributes [20]. As the estimate of the classifying importance of a set of the properties of elements, we used the ratio of the accuracy of recognition of a control sample for an initial set of properties of elements to the accuracy of recognition performed without regard for the set of properties to be estimated.

As a result of solving each of the three classification problems, we formed the corresponding samples for the subsequent computer training. For describing compounds, they included the following samples:

sample 1, only an initial set of properties of elements;

sample 2, only the properties of elements that are most important for classification and were chosen by a computer with the computer program [20];

sample 3, an initial set of properties of elements and the most important algebraic functions of these properties chosen by a computer.

Choice of Algorithms for Computer Data Analysis

For computer data analysis, we used the set of precedent-based pattern recognition algorithms that was included into IAS developed by us [25]. At present, this system unites programs based on estimate calculation algorithm, the method of binary decision trees, a linear Fisher discriminant, LoReg, searching for logic regularities for classes, searching for two-dimensional linear separators, linear machine algorithm, various versions of neural network training, k nearest neighbor method, dead-lock test selection, support vector machine, statistically weighed syndromes, formation of concepts using growing pyramidal networks, and so on [26, 27]. When solving each specific problem using various sets of properties of elements, we chose the most accurate algorithms. To this end, we used examination recognition with cross-validation for a training sample, which is a traditional means to estimate the quality of computer training [26].

To increase the accuracy of predicting the formation and the type of crystal structure of compounds, we used the strategy of collectives of algorithms [26]. The following algorithms of constructing collective solutions were included in IAS: the Bayes method, clustering and selection algorithm, decision templates, the dynamic Woods method, combined committee methods, logic correction, convex stabilizer, generalized polynomial corrector, and algebraic corrector. As a rule, the use of the strategy of collective algorithms can improve the prediction accuracy due to mutual compensation of the

disadvantages of one algorithm by the advantages of others.

To estimate the accuracy of algorithm collectives, we applied examination recognition of 100 examples, which were randomly selected from training samples and were not used in computer training (at the final stage of prediction, the control examples were returned to a training sample).

Prediction of the Formation and the Type of Crystal Structure of Equiatomic Silicides and Germanides

The chosen most important sets of properties were used for computer training to search for classifying regularities. For training, we used the most accurate methods of pattern recognition and collective decision making. The final result was formed by comparing the predictions obtained upon solving the three classification problems. If the results contradicted each other, the prediction was considered to be indefinite and an empty cell was placed in the corresponding table of predictions. It should be noted that, to predict new equiatomic compounds, we only used the properties of the chemical elements forming their composition.

RESULTS AND DISCUSSION OF COMPUTER EXPERIMENTS

Based on an analysis of the information from database "Phases" on the properties of inorganic compounds [21], we formed a sample containing 222 examples of ABX (X = Si or Ge) compounds with a TiNiSi-type crystal structure under standard conditions, 34 examples of equiatomic compounds with a ZrNiAl-type crystal structure, 70 ABX compounds with a PbFCl-type crystal structure, 269 compounds with structures other than those given above, and 64 examples of systems without the formation of equiatomic compounds. When solving various classification problems, we also used information on the compounds for which, e.g., only crystal system or formation possibility was determined.

We found that the functions $M(A) \times M(B)$ and $I(A) \times I(X)$, where M is the Mendeleev–Pettifor number of elements A or B [23, 24] and I is the thermal conductivity of element A or X, are most important to classify systems in the sign of formation or absence of equiatomic compounds and the functions $T(A) + T(B)$ and $I(A)$, where T is the melting temperature of element A or B and $I(A)$ is the thermal conductivity of element A, are the most strongly separating parameters for crystal-chemistry classification into five classes. Last parameters also determined the separation of the experimentally studied compounds with a TiNiSi-type crystal structure from the examples of compounds with other crystal structures and the examples of systems without the formation of equiatomic phases. Parameters $M(A) \times M(B)$ and $I(A) \times I(X)$ were the most important classification parameters for solving the problem in the case where compounds with ZrNiAl and PbFCl structures served as target classes.

The problem of the sufficiency of the chosen parameters for a correct classification of equiatomic phases in the sign of the formation and type of crystal structure was resolved by computer experiments on estimating the accuracy of computer training using various sets of the properties of elements (see samples 1–3) for the same experimentally studied substances.

The calculations show that the use of the most important parameters of elements for classification in predicting the formation of equiatomic silicides and germanides gives the best result in most cases (up to 96%) for many pattern recognition algorithms (except for the binary decision trees, LoReg, and k nearest neighbor methods). Other results were obtained for predicting the type of crystal structure. When solving problem 2, in most cases (more than 78%) we obtained the best prediction results when using the set that includes the initial properties and the algebraic functions of the initial properties that are most important for classification (except for the training algorithms of neural networks and the calculation of estimates and statistically weighed syndromes). In most cases, the use of only the most important parameters of elements chosen by a computer yields much worse results (below 61%). In all cases, the application of only the "good" classifying parameters in solving problem 3 decreased the prediction accuracy. The addition of the algebraic functions most important for classification to the initial set of properties also not always improved the prediction quality.

Based on an analysis of the examination recognition results, we can conclude that the use of only the properties of elements that are most important for classification for prediction not always leads to correct results. In most cases, only rough separation of the points corresponding to substances of different classes can be obtained on the projections on planes the coordinates of which are separate (even most important for classification) properties or functions of these properties. A "finer" classification, which takes into account the specific features of different substances, can be obtained with a multidimensional model, which includes a wide spectrum of properties of components in combination with the most classifying parameters, namely, the algebraic functions of the initial properties.

To improve the prediction accuracy further, we performed computer experiments on searching for effective methods for collective decision making using the most accurate algorithms of precedent-based pattern recognition. Hundred-per-cent examination recognition in predicting the formation of equiatomic silicides and germanides was obtained for the set of properties of elements that included the initial properties and the algebraic functions of the properties of elements that are most important for classification during the application

Table 1. Predicted types of crystal structure of *AB*Si compounds

B \ *A*	Ca	Sc	Ti	V	Cr	Mn	Sr	Y	Zr	Nb	Ba	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu	Hf	Ta	Th	U
Mg	#1	1					#1	1		1	#3					1	1	#1	1	1	1	1	1	1	#1	1				1
Al	#4	4				5	#4	4		1	4	4	4	4	4	4	4	4	4	4	4	4	4	4	4	4	1	1	4	4
Ti	3	3		5	5	5	3	3		#5						3		3	#3	#3	3	3	#3	3	3	#3	#5		3	
V						5		3	#3	5			#5			3		3	3	3	3	3	3	3		3	#3			
Cr			1					3	#1	#2			#5					3	3								#1	1		
Mn	#3	#2	#2		4		3		#1	#2	3	#3	#3	#3	#3	3	#3	3	#3	3			#1	#1		#1	#1	#2	4	
Fe	#5	3	#4		#4	#5		#3	#1	1		#3	#3	#3	#1	3	#3	3	#3	#3	#3	#3	#3	#3	#3	#3	#1	#1		
Co		#1	#1	#1	#1	#1		#1	#1	#1		#3	#3	#3	#3	3	#3				1	#1	#1	#1		#1	#1	#1	#4	
Ni	#4	#1	#1	#1	#1	#1	4	#1	#1	#1	4	#4	#4	#4	#4	4	4		#1	#1	#1	#1	#1	#1	1	#1	#1	#1	#4	4
Cu	#4	#2	#1			#5	#4	#4	#1	1	4	#4	#4	#4	#4	4	#4	#4	#4	#4	#4	#4	#4	#4	#4	#4	#1	1	4	4
Zn	#4	4				5	#4	4		1	#4	4	4	4	#4	4	4	#4	#4	4	4	4	4	4	4	4		1	4	4
Y	4	4					0				3					4		4	4	4	4	4	4	4	4	4				
Ru		1	#4		1	1		#1	#2	#4		#3	#1	#3	#3	3	#3	3	#3	#1	#1	#1	#1	#1	1	#1	#1	1	4	#1
Rh		#1	#1	1	1	#1		#1	#1	#1		#4							#1	#1	#1	#1	#1	1	1	#1	#1	#1	4	1
Pd	#4	#1	#1	1	1	1	#4		#1	1	#4	4	#4	4	#4	4	#4	#4	#4	#4	4						#1	1	4	4
Ag	4	#2		2			4	#2			4	#4	#4	#4	#4		#2		#2	2	#2	2	#2	#2	#2	#2			4	
Cd	4	2	1			5	4	4	1	2	4	4	4	4	#4	4	4	4	4	4	4	4			4	4	1	1	4	4
W	3	1					3			#5	3	3	3	3	3	3	3	3	3					1	1	1	#1			
Re			#2						#2	#2	3	3	3	3	3					1	1	1	1	1		1	#2	#4	4	
Os	3	1	#1	1	1	1	3	1	#1		3	3	#3	3	3	3	3			1	1	1	1	1	1	1	#1		4	1
Ir		#1	1	1	1	1	4	#1	#1	#1	4	#4	#4	#4	#4		4	1	#1	#1	#1	#1	#1	#1	#1	#1	#1	#1	#4	
Pt	#4	#1	#1	1	1	1	#4	#1	#1	#1	#4	#4	#4	#4	#4	4	#4	#4	#4	#1	#1	#1	#1	#1	#1	#1	#1	#1	#4	4
Au	4	#4					4	4	0	1	4	4	4	4	#4	4	4	4	4	4	4	4	4	4	#4	4	1	1	#4	4

Table 2. Predicted types of crystal structure of *AB*Ge compounds

B \ *A*	Na	Mg	Ca	Sc	Ti	V	Cr	Sr	Y	Zr	Nb	Ba	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	To	Dy	Ho	Er	Tm	Yb	Lu	Hf	Ta	Th	U
Mg			#1	1	1			#1	1	1		#3					1	1	#1	1	1	1	1	1	1	#1	1	1	1		
Al	#3	#5	4	4	5	0		#4	4		1	#4	4	4	4	4	4	4	4	4	4	4	4	4	4	4	4		1	4	4
Ti		3	3	3				3	#3				#3	#3	#3	#3	3	#3	3	3	3	#3	#3	#3	#3	3	#3	5	5	3	3
V		3	3		4		4	3	3	#4	4		3	3	3	3	3	3	3	3	3	3	3	3			3	4		3	3
Cr	3	3	3		4	4		3		4	#4	3	3	3	3	3	3									4					0
Mn	3	#3	#3	#2	1	2	4	3		#1	#2	3	#3	#3	#3	#3	3		1	#1	#1	#1	#1	#1	#1	#4	1				
Fe	3	3	3	#2	#4		4	3	3	#1	#4	3	3	3	3	3	3	3						1	1	#4	1	#2	#1		3
Co	3	#3	3	#1	4	#1	1	3	1	#1	#1	3	#3	#3	#3	#3		#1	1	#1	#1	#1	#1	#1	#1	#1	#1	#1	#1		1
Ni	3		#3	#1	#1	#1	1		1	#1	#1	4		#1	#1	#1	1	#1	#4	#1	#1	#1	#1	#1	#1	#1	#1	#1	#1	1	#1
Cu	4	#3	#4	#2	#1	1		4	#4	#1		#4	#4	#4	#4	#4	4	#4	#1	#4	#4	#4	#4	#4	4	#4	#4	#1	1	4	
Zn	4	0	#4	4	1		4	#4	#4	1		#4	#4	#4	#4	#4	4	#4	#4	#4	#4	#4	#4	#4	#4	#4	4	1	1	4	4
Y		4		4	4			4		4	4		4	4	4	4	4	4	4	4	4	4	4	4	4	4	4	4	2	4	4
Ru				#2	#4	2	4	3	1	#4	1		#3	#3	#3	#3	0		1		1	#1	#1	#1	#1	1	#1	#4	4		
Rh				2	#4		4	4	#1		1	4	4	#1	#1	#1	1	#1	1	#1	#1	#1	#1	#1	#1	#1	#1		1	1	
Pd	4	0	4	#2	#1	1		4	#4	1	1	4	#4	#4	#4	#4	4	#4	#4	#4	#4	#4	#4	#4	#4	#4	4	1	1	4	4
Ag		0	#4	#2			2	4	#2			4	#4	#4	#4	#2		#2	#4	#2	#2	#2	#2	#2	#2	#2	#2			4	
Cd		0	#2	2	1			#1		1		#4	4	4	4	4			#1		4	4			2	#2	2	1	1	4	4
W			3	2				3				3	3	3	3	3	3														
Re			3	2				3				3	3	3	3	3	0														
Os			3	#2	#4	4	4	3		#4		3	3	3	3		3				1	1	1	1	1	1	1	#4		4	
Ir			1	#1	4	4	4		#1	#1	#1	4	#4	#1	#1	#1	1	#1	1	#1	#1	#1	#1	#1	#1	#1	#1	#1	1		4
Pt	4	1	#1	#1	1	1		#4	#1	#1	1	#4	#4	#4	#4	#4	4	4	#4	#1	#1	#1	#1	#1	#1	#1	1	#1	1	4	#4
Au	#4		4	#4			4	4	#4	4	1	4	#4	#4	#4	#4	4	#4	#4	#4	#4	#4	#4	#4	#4	#4	#4			4	#4

of pattern recognition methods such as training based on binary decision trees, neural network training, the *k* nearest neighbor method, and the Bayes method of collective decision making. During the prediction of the type of crystal structure (five classes), the best results were obtained for the initial set of properties of components during the application of conventional majority voting for the pattern recognition algorithms, namely, the linear machine, the neural network, and the *k* nearest neighbor algorithms. When using algorithm collectives, we were able to increase the prediction accuracy by more than 20%. The accuracy of prediction of the TiNiSi-type crystal structure of *ABX* compounds was also increased due to the use of collective algorithms (linear machine, support vector machine, neural network, LoReg, *k* nearest neighbors) and the Bayes method for decision making. In this case, to describe compounds, we also used the algebraic functions of the properties of elements that are most important for classification along with the initial set of properties of elements.

The application of only the initial properties of elements and majority voting in analyzing the results of examination recognition of 100 randomly chosen substances obtained with the use of the of linear machine, neural network training, and *k* nearest neighbor algorithms was most efficient for predicting ZrNiAl-type crystal structures. The committee method (averaging) for the set of pattern recognition algorithms (linear machine, neural network, LoReg, *k* nearest neighbor) and taking into account the set of properties of elements that includes the initial properties and the algebraic functions of the properties of elements that are most important for classification allowed us to improve the accuracy of predicting the PbFCl crystal type structure of equiatomic silicides and germanides.

Tables 1 and 2 present the data of predicting new *AB*Si and *AB*Ge compounds. The following designations are used: 1, 2, 3 stand for the prediction of *ABX* compounds with TiNiSi-, ZrNiAl-, and PbFCl-type crystal structures, respectively, under standard conditions; 4 is the prediction of *ABX* compounds with a crystal structure other than these structures; 5 is the prediction of the absence of an equiatomic compound in an *A*–*B*–*X* system; and symbol # designates the well-known systems information on which was used for computer training. The empty cells correspond to a discrepancy between the predictions obtained in solving these three classification problems.

CONCLUSIONS

(1) Using special-purpose programs of computer analysis of information on the well-known equiatomic *ABX* (*A* and *B* are various metals, *X* = Si or Ge) compounds, we found that the functions that are most important for classifying systems in the sign of formation or absence of equiatomic compounds were $M(A) \times M(B)$ and $I(A) \times I(X)$, where *M* is the Mendeleev–Pettifor number of element *A* or *B* and *I* is the thermal conductivity of element *A* or *X*, and that the parameters that most strongly separate compounds for crystal chemical classification were functions $T(A) + T(B)$ and $I(A)$ (where *T* is the melting temperature of element *A* or *B*), $I(A)$, $M(A) \times M(B)$, and $I(A) \times I(X)$.

(2) As a result of computer experiments on estimating the accuracy of computer training using the well-known compounds as examples, we solved the problem whether the chosen parameters are sufficient for a correct classification of equiatomic phases in the sign of formation and the type of crystal structure. It was shown that the most accurate results can be obtained using a wide set of the properties of elements and the algebraic functions of these properties that are most important for classification. The search for such complex classifying dependences is possible when the methods of precedent-based pattern recognition are used. With these methods, we found the criteria that can be used to divide *A*–*B*–*X* systems into systems with and without formation of equiatomic compounds and to classify *ABX* compounds in the type of crystal structure using only the parameters of the elements.

(3) Using the found criteria, we were able to predict new equiatomic silicides and germanides and their types of crystal structure under standard conditions. An analysis of the predictions showed that most new compounds have TiNiSi- and PbFCl-type structures.

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