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# Prediction of intermetallic compounds

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**Abstract. The problems of predicting intermetallic compounds not yet synthesized are discussed. It is noted that the use of classical physicochemical analysis in the study of multicomponent metallic systems is associated with the complexity of presenting multidimensional phase diagrams. The use of modern information technology with application of computer pattern recognition method is a route to the prediction new intermetallics with specified properties. The algorithms used most often in these methods are briefly considered and the efficiency of their use for predicting new compounds is demonstrated. The bibliography includes 144 references.**

## I. Introduction

Physicochemical analysis founded by Academician N S Kurnakov [1] remains at present the main scientific method for the design and investigation of the structural and functional inorganic materials. The progress in the physicochemical analysis is associated with the involvement of methods and approaches developed in such areas as theoretical physics, quantum chemistry, crystal chemistry, as well as the application of modern information technologies. The development of the theoretical methods for prediction of new phases with preset properties and the subsequent synthesis of these phases and experimental verification of the prediction can become one of the effective trends.

In the present review, the possibilities of such an approach are considered and the results of the experimental verification of predictions for specific examples of the intermetallics are given. The latter are chosen as subjects for the investigation as a promising base for the functional materials of the new generation.

The physicochemical analysis is at the front line of a complex of methods used in physical metallurgy.[2] One can make important conclusions and certain generalizations using physicochemical analysis based on the results of relatively simple physical measurements. The geometric analysis of the phase diagrams of chemical systems gives vast information on the nature of metallic phases and conditions of their formation. The nature and composition of the phases formed in a system are investigated using physicochemical analysis without recourse to their isolation (in contrast to the preparative methods). This approach is based on the investigation of the functional dependences of the properties of a chemical equilibrium system on the factors that define its equilibrium state.[3]

At present, thousands of phase diagrams of binary and ternary metallic systems have been studied, the relevant data are given in the reference books by both Russian † and foreign authors,[4–10] as well as in the databases on phase diagrams.[11–13] The development and application of the computer databases on the properties of inorganic compounds and materials is a new and promising trend for the acquisition, analysis and on-line delivery to the specialists of information on phase diagrams and properties of the phases formed. These databases contain huge data, which are indispensable for the design of new materials of the construction and functional purposes. Table 1 lists some databases on the properties of inorganic materials.

Certain difficulties emerge in the investigation of multicomponent systems. The geometric methods of the state diagram representation become improper: even in the case of three-component systems, one has to use polythermal and isothermal sections, which provide precise data only for fixed temperatures and compositions. Even greater difficul-

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† Among latest publications one should mention the multivolume reference book 'Phase Diagrams of Binary Metallic Systems' (Ed. N P Lyakishev) (Moscow: Mashinostroenie, 1996 – 2000).

**Table 1**. Databases on the properties of inorganic compounds and materials.

| Name and subject field | Organization | Country | Ref. |
|---|---|---|---|
| Databases on the phase diagrams of inorganic systems | | | |
| 'Diagram', database on phase diagrams of the systems with semiconductor properties | A A Baikov Institute of Metallurgy and Materials Science RAS | Russia | 11 – 16 |
| 'Pauling File on Binary Systems', database on phase diagrams of binary systems and crystal structure of binary compounds | Japan Science and Technology Corporation;<br>National Institute of Materials Science;<br>The University of Tokyo<br>Material Phases Data System | Japan<br><br><br>Switzerland | 17, 18 |
| Database on the thermal and thermodynamic properties of inorganic compounds and materials | | | |
| 'IVTANTHERMO', database on the thermodynamic properties of individual compounds | Institute of Thermophysics of Extreme States of the Joint Institute for High Temperatures RAS | Russia | 19, 20 |
| 'NISTTHERMO', database on the thermodynamic properties of compounds | National Institute of Standards and Technology | USA | 21 |
| 'NIST/TRC Ideal Gas DB', database on the ideal gases | " | " | 22 – 25 |
| 'JANAF', database on the thermochemical properties of compounds with one or two carbon atoms | " | " | 26 |
| 'THERMODATA', database on the thermodynamic properties of inorganic compounds | THERMODATA | France | 27 |
| 'MTDATA', database and programme package for the calculation of phase equilibria and thermodynamic properties of the multicomponent systems | National Physical Laboratory | Great Britain | 28, 29 |
| 'JICST TH', database on the thermophysical and thermochemical properties of compounds | Japan Information Center of Science and Technology | Japan | 30 |
| 'TPRC/TPMD', database on the thermophysical properties of compounds | Center for Information and Numerical Data Analysis and Synthesis of Purdue University | USA | 31 |
| 'SGTE', database on the thermodynamic properties of inorganic compounds | Scientific Group Thermodata Europe | EU | 32, 33 |
| 'THERMO-CALC', thermodynamic database and programmes for the thermodynamic calculations | Thermo-Calc Software Inc. | Sweden | 34 – 36 |
| 'THERSYST', database on the thermophysical properties of alloys | Institute for Nuclear Energy and Energy Systems of University of Stuttgart | Germany | 37 |
| 'NEA-TDB', database on the thermophysical properties of actinide derivatives and other compounds for nuclear energy | Nuclear Energy Agency | France | 38 |
| 'F*A*C*T', database on the thermodynamic properties of inorganic compounds | Ecole Polytechnique de Montréal; McGil University; Centre for Research in Computational Thermochemistry | Canada | 39 |
| 'CompoTherm', database and prediction system on the thermophysical properties of composites | National Institute of Materials Science | Japan | 40 |
| Databases on crystal chemistry and crystal structures | | | |
| 'ICSD', database on the crystal structures of inorganic compounds | Fachinformationszentrum Karlsruhe<br>National Institute of Standards and Technology | Germany<br>USA | 41 – 46 |
| 'EDD', electron diffraction database | National Institute of Standards and Technology;<br>Sandia National Laboratory | " | 47 – 50 |
| 'CRYSTMET', database on the crystal structures of intermetallic compounds | TOTH Information Systems, Inc. | Canada | 51 – 53 |
| 'Mincryst', database on crystallography and crystal chemistry of minerals and their structural analogues | Institute of Experimental Mineralogy RAS | Russia | 54 |
| 'PDF', database on powder diffraction patterns of inorganic and organic compounds | International Center for Diffraction Data | USA | 55 – 57 |

**Table 1** (continued).

| Name and subject field | Organization | Country | Ref. |
|---|---|---|---|
| Databases on physical properties of inorganic compounds and materials | | | |
| 'Phases', database on the properties of inorganic compounds | A A Baikov Institute of Metallurgy and Materials Science RAS | Russia | 11, 14, 15, 58 |
| 'Crystal', database on the properties of compounds with particular acousto-optical, electro-optical and non-linear-optical properties | " | " | 11, 14 – 16, 59, 60 |
| 'Bandgap', database on the forbidden zone widths of inorganic compounds | " | " | 14, 15 |
| 'Elements', database on the properties of chemical elements | " | " | 15 |
| 'SMET', database on the properties of materials for electronics | A V Nikolaev Institute of Inorganic Chemistry, Siberian Branch of RAS | Russia | 16, 61 |
| 'SSD', surface structure database | National Institute of Standards and Technology | USA | 62 |
| Database on the physicochemical properties of high-purity substances | Institute of Chemistry of High-purity Substances RAS | Russia | 16, 63 |
| 'DIPPR', database on properties of the temperature-dependent industrial compounds | Design Institute for Physical Property Data of the American Institute of Engineers | USA | 64 – 68 |
| 'SUPERCON', database on the properties of superconductors | National Research Institute for Metals | Japan | 69 |
| 'ADAMIS', database on the properties of alloys for microsolders | University of Tohoku | " | 70 – 72 |
| Database on the properties of rare-earth metals | Institute of Applied Chemistry of Academia Sinica (Changchun) | China | 73 |
| 'HYDROGENE DATA', database on the properties of hydrogen-containing materials | Centre National de la Recherche Scientifique; Centre d′Etudes de Chimie Metallurgique | France | 74 |
| Database on the phosphor properties | Research and Manufacturing Association 'Phosphor' | Russia | 75 |
| 'EPIDIF', database on the coefficients of interdiffusion of the components of gas phase epitaxy of semiconducting materials | Joint Institute of High Temperatures RAS | " | 76 |
| 'MAT-DB', database on the mechanical and physical properties of industrial alloys | Joint Research Centre of the European Commission Institute of Energy | Netherlands | 77 |
| 'SPTD1', database on the structural phase transitions | Institute of Low Temperature and Structural Research of PAN | Poland | 78 |
| 'JMPD', database on the materials for nuclear energetics | Japan Atomic Energy Research Institute [a] | Japan | 79 |
| 'Data-Free-Way', system of databases on nuclear materials | Japan Atomic Energy Research Institute; [a] National Institute for Materials Science; Japan Nuclear Cycle Development Institutea | " | 80, 81 |
| Database on the functional ceramic materials | University College; Imperial College; University of London; Regional Research Laboratoty | England India | 82 |
| Database on the incommensurate phases | Universite Catholique de Louvain | Belgium | 83 |

[a] In 2005, the organization joined the Japan Atomic Energy Agency.

ties emerge in the case of quaternary and more complex systems. In addition, studies of multicomponent systems require laborious experimental work and substantially greater consumption of materials, including expensive ones. The ways to reduce the cost of the investigation of such systems have been suggested.[84, 85] One of them is the *a priori* prediction of new inorganic phases with predefined properties [11] using modern computer technologies.

## II. Methods for the *a priori* prediction of new intermetallic phases

The objective of the *a priori* prediction of not yet synthesized intermetallic compounds can be formulated [11] as the search for the combination of chemical elements and their ratio (*i.e.*, determination of qualitative and quantitative compositions) for the synthesis (under given ambient con-

ditions) of a certain crystal structure of a substance that possesses the required functional properties. It is the knowledge of the properties of chemical elements and the compounds already studied that constitute initial information for the prediction of intermetallic compounds. The problem of the design of new intermetallic compounds can be reduced to the discovery of the relationships between the properties of the metallic systems (including properties of the substances) and the properties of elements that form these systems. We shall now consider possible methods for the prediction of the intermetallic compounds.

It should be reminded that the metallic systems are among the primary subjects for the physicochemical analysis.[1] In the state-of-the-art physicochemical analysis, the concepts of topology, diagram metrics for the chemical systems and thermodynamic calculations go well together with experimental investigations, so it is considered to be the main tool for the investigation of the phase diagrams. However, in the majority of cases, one cannot *a priori* predict the possibility of the formation of intermetallic compounds solely with the help of theoretical methods of physicochemical analysis (except for those that are the result of the phase rule). Special expectations were placed on the quantum mechanical methods of calculations, which provide, in principle, the possibility of prediction of new intermetallics. However, because of mathematical difficulties encountered in the application of the calculation methods for such complex systems as intermetallic compounds in the solid state, one can obtain only approximate solutions.

By now, huge information has been collected on the properties of metallic and other (non-metallic) inorganic compounds. It is evident that the recurring relationships exist between properties of compounds and properties of elements constituting them. Moreover, the known compounds should follow these rules. Hence, the search for the rules of the formation of certain types of compounds based on the analysis of information on the synthesized compounds is realistic. Dependences found can be applied for the predictions of unknown compounds using only information on the properties of their constituents. It is this idea that was the basis of the computer simulation of not yet synthesized inorganic compounds.[11]

The methods for prediction of intermetallic compounds based on the usage of special softwares for pattern recognition in order to find correlations between information stored in the databases containing properties of inorganic compounds and materials and results of their application are considered below.

## III. Methods and algorithms for the prediction of intermetallics based on the computer pattern recognition method

The first investigations into the application of the pattern recognition methods for the prediction of intermetallic compounds were carried out by Savitskii and his co-workers in the mid-1960s.[86] The results of the prediction for rather simple binary phases turned out to be excellent: their comparison with the obtained experimental data showed that the reliability of the prediction of the binary compounds exceeded 90%.[87,88]

Using machine learning methods of pattern recognition for the prediction of intermetallic and other inorganic compounds, the problem can be defined as follows. Let the space of properties of the elements that constitute the chemical systems (the so-called feature space) is given. This space contains fixed number of regions corresponding to different classes of such systems. The borders of the regions are not defined and the rules are absent that could assign the points (objects) corresponding to the chemical systems to one or another region. During learning, points from these regions ‡ are transferred to the computer system together with information as to which region these points belong. The goal of learning is to build the surfaces (classification criteria) that separate not only the known, but also all other points belonging to these regions. In the course of the prediction, only the coordinates (the set of the properties of chemical elements) of a point that corresponds to a system yet to be studied are presented to the computer, and the computer system defines to which class of chemical systems the one predicted belongs.

What classes of chemical systems are usually studied? These could be the systems with and without formation of compounds (eutectics, solid solutions, *etc*.), the systems with and without formation of compounds with the predetermined component ratio and/or with a preselected crystal structure type under the given ambient conditions, the systems with and without formation of compounds with the predetermined functional properties (*e.g*., melting point or superconducting transition temperature higher or lower than a certain value, *etc*.).

There are many algorithms of computer learning to pattern recognition. Simple algorithms were used at the dawn of the implementation of the pattern recognition methods in metal science that did not require resource-intensive operations, which was associateded with low computer performance. For example, softwares developed by Devingtal'[89,90] were used in the pioneering studies on the design of binary intermetallic compounds where linear programming has been used for the solution of the extremal problems of pattern recognition. In later papers by Vozdvizhenskii and Falevich,[91,92] an algorithm of potential functions was used for the prediction of binary metallic systems using the interaction type of the components in a liquid state.[93] The estimate calculation algorithms[94] was applied[95] to the search for optimal quantities of additives of different chemical elements to the steel for attaining the extreme mechanical properties. A linear algorithm of computer learning of pattern recognition was applied[96] to the search for alloy dopants. Mechanical properties of steels were predicted[97] with the application of the algorithm of binary decision trees (see[98]). The discriminant analysis was widely used for the prediction of the possibility of the formation of binary compounds with lanthanides,[99,100] of the crystal structure type for refractory binary compounds with different compositions,[101] of the type and concentration of defects and of defect formation energetics in imperfect crystals of refractory compounds.[102]

Algorithms based on the associative organization of the computer memory in the form of the artificial neural[103–106] or growing pyramidal[107] networks are among the most popular. Their application allowed the solution of numer-

‡ This is referred to as the training set. Such a set includes examples from the systems already studied that are represented in the computer memory as an array of value of properties of the chemical elements that constitute the system.

ous problems on the prediction of the possibility of the formation, crystal structure type and properties of intermetallic and other inorganic compounds.[11, 88, 108–126] The target classification criterion formed by these algorithms has a form of a 'trained' network.[103–107] The possible reason for the successful application of the network algorithms for the solution of complicated problems of the prediction of inorganic compounds is that the network stores not only the borders between classes or certain reference points of different classes, but also the regions as a whole that correspond to a certain class of systems, the form of these regions in the multidimensional space of the element properties being rather complicated. The effective application of this type of algorithms was favoured by the significant increase in computer performance so that the time of the network learning decreased substantially. In addition, standard programme packages were developed, for example, BrainMaker (Loral Space), OWL (Hyper-Logic), The All Trilogy (Ward Systems Group), Neural Connection (SPSS Inc.), Statistica: Neural Networks (Stat-Soft Inc.), *etc*., where the neural network algorithms are implemented.[106] Significant problems in the application of such algorithms are the availability of huge files for the training of the neural network as well as the effect of overfitting of the neural network when it works well with the training set, but poorly predicts new objects. The same problems are encountered in the application of the algorithms based on the support vector machines, which is commonly used in chemical applications.[127–129]

The latest trend is the development of special information-analytical systems for computer-assisted design of chemical compounds, which include databases on the properties of compounds and materials as well as the programmes for the search of regularities in the data arrays and for the prediction. As an example, we shall discuss the structure of the information - analytical system developed in IMET RAS (Fig. 1),[130] which is widely used for the design of not yet synthesized inorganic compounds. It includes an integrated system of databases on the properties of inorganic compounds and materials[11–16, 58–60] and the programme package for pattern recognition.[107, 131]

The system of the regularly updated databases on the properties of inorganic compounds and materials at present comprises the following information subsystems (Fig. 2):

— databases that contain brief information on the most common properties of inorganic compounds and chemical elements: (1) database on the properties of inorganic compounds 'Phases',[11, 58] which contains information on the properties of 45 000 ternary and more than 15 000 quaternary compounds retrieved from 23 000 literature sources; (2) database on the properties of the chemical elements 'Elements',[15] which includes data on more than 90 parameters for each element;

— specialized databases that contain detailed information on the properties of compounds and materials important for their applications: (1) database 'Diagram'[11–14] on the phase diagrams of semiconductor systems with information collected and examined by highly skilled experts on phase diagrams of semiconductor systems and on physicochemical properties of the phases formed in the systems; this database contains detailed information on several tens of

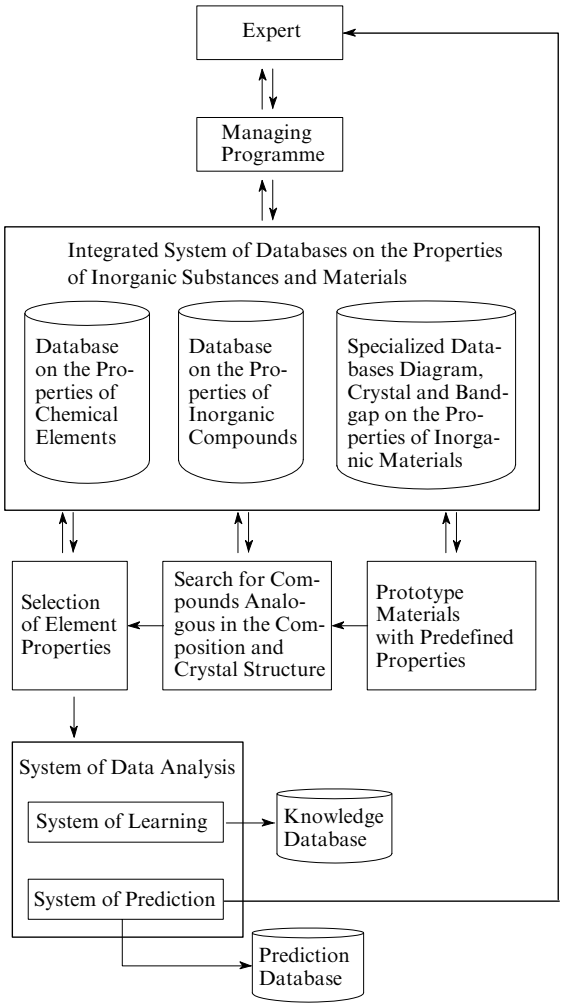



**Figure 1.** Flow chart of the information-analytical system for the design of inorganic compounds.

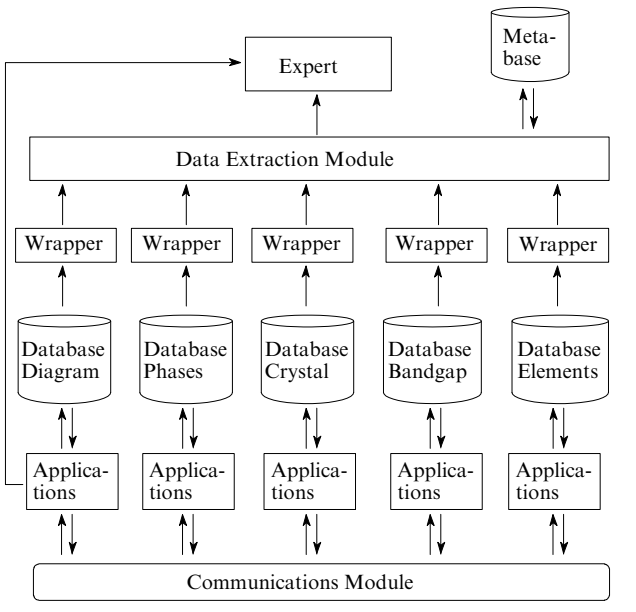



**Figure 2.** Flow chart of the integrated system of databases on the properties of inorganic substances and materials of the IMET RAS.

systems important for the semiconductor electronics; (2) database 'Crystal'[11, 14, 60] on acousto-optical, electro-optical and non-linear optical properties of compounds, which contains information on the parameters for more than 100 materials; (3) database 'Bandgap'[14] on the forbidden zone widths of inorganic compounds, which at present contains data for more than 3 000 substances.

The cumulative volume of databases in the integrated system of the information-analytical system of the IMET RAS is ~8 GB.§ The integrated system of databases allows specialists to obtain information on the properties of compounds and materials directly from different databases.

The data analysis subsystem of the information-analytical system contains the following programme learning methods for the computer pattern recognition.

(1) A wide class of algorithms of the Recognition system developed at the Computer Centre of the RAS.[131] This multifunctional system for pattern recognition, in addition to the well-known algorithms of the linear machine, Fisher's linear discriminant, *k*-nearest neighbours, support vector machine, neural network and genetic algorithms, includes also estimate calculation algorithms, the deadlock test algorithm, the terminal test algorithm, the algorithm of logical regularities, algorithm of the statistical weighted syndromes, *etc*.

(2) The computer learning system ConFor[107] for the concept formation mechanism, which is based on a special data structure in a computer memory as growing pyramidal networks.

The information-analytical system of the IMET RAS allows the solution of two important problems. First, the partial automation is possible of the analysis of huge experimental chemical information when searching for the regularities necessary for the subsequent design of new compounds with predetermined properties. Second, the potential of the conventional databases on the properties of compounds and materials are expanded, since the user gets an access to not only information on the substances already investigated, but also the prediction of the compounds not yet synthesized and estimation of their properties based on earlier predictions. The advantage of the developed information-analytical system is that it is available through Internet (http://ias.imet-db.ru), which enables quick on-line link to alive data and regularities.

## IV. Results of the predictions of new intermetallic phases

The results of the prediction[119–124] are compared with newer experimental data to demonstrate the potential of the computer learning methods for the pattern recognition in the computer design of intermetallic compounds. The prediction error is evaluated as the ratio of the incorrectly predicted objects to the total number of the results tested.

### 1. Compounds with the composition $AB_2X_2$ (X = Al, Si, Ge, P, As, Sb) and the crystal structure of the $ThCr_2Si_2$ type

The prediction of compounds not yet synthesized with the composition $AB_2X_2$ (hereinafter, A and B are different chemical elements; X = Al, Si, Ge, P, As, Sb) with tetragonal structure of the $ThCr_2Si_2$ type was performed.[120–123] Such compounds are promising in the search for new magnetic materials.[132–135]

The data arrays for the computer learning with the programme ConFor[107] included several hundreds of examples of the formation of phases with the crystal structures of the $ThCr_2Si_2$ type under ambient conditions and hundreds of examples of the absence of compounds with this crystal structure in the A–B–X systems. Learning and prediction were carried out separately for each type of compounds. For the systems with X = Al, P, As, Sb, in addition to the phases with the structure of the $ThCr_2Si_2$ type, new compounds with the structure of the $CaAl_2Si_2$ type were predicted.[120, 121]

For the representation of the A–B–X systems in the computer memory, the following sets of properties (spaces) of elements A and B were used:

I — electron distribution over the energy shells of the isolated atoms;

II — first three ionization potentials, metal radii, standard entropies of the individual compounds, melting points, the number of completely filled electron shells, the number of electrons on the incompletely filled s-, p-, d- and f-shells of atoms.

The computer training and prediction were performed for each set of properties of the element and for each group of the A–B–X systems with different components X. Predictions based on two sets of properties for compounds of a given system should coincide due to the statistical correlation of the element properties. The results of the prediction with the application of both sets of the element properties for each group of compounds with X = Al, Si, Ge, P, As, Sb were compared and the decision was made on the assignment of a compound to the class of phases with the structure of the $ThCr_2Si_2$ type (or $CaAl_2Si_2$ one), when the results of the prediction did not contradict each other.

The results of the experimental verification of the predictions for the compounds with the compositions $AB_2Si_2$ and the $AB_2Ge_2$ obtained with the use of the two above-mentioned sets of properties of the elements are given in Tables 2 and 3.

Table 4 contains results of the comparison of the predictions for the compounds with the composition $AB_2P_2$ with the newer experimental data.

For the silicides, 89 compositions have been experimentally tested and only in six cases the results turned out to be incorrect, *i.e*., the prediction error was 7%. For the germanides, 49 compositions have been tested and in six cases, too, the predictions did not coincide with the experiment, *i.e*., the prediction error is equal to 12%. For the phosphides, 10 compounds were synthesized and only one prediction was incorrect (the prediction error is 10%). The average error of the prediction of the type of crystal structures for compounds with the composition $AB_2X_2$ (X = Al, Si, Ge, P, As, Sb) was 8%.

### 2. Compounds with the composition ABX (X = Al, Si, P, Ga, Ge, As, Pd, Sb, Bi)

The prediction of the crystal structure type for the equiatomic compounds ABX (X = Al, Si, P, Ga, Ge, As, Pd, Sb, Bi) under ambient conditions was carried out.[119–121] Phases with the hexagonal structure of the ZrNiAl type and with the orthorhombic structure of the TiNiSi type were predicted for the compounds with aluminium, germanium and

§ The system is available on-line to the registered users (http://www.imet-db.ru).

**Table 2**. Examples of the prediction of compounds with the composition $AB_2Si_2$ with crystal structure of the $ThCr_2Si_2$ type.[123]

| Element A | Element B | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | Cr | Mn | Fe | Co | Ni | Cu | Zn | Ru | Rh | Pd | Ag | Os | Ir | Pt | Au |
| Ca | + | ⊕ | ↔ | ⊕ | ⊕ | ⊕ | ⊕ | + | + | © | ⊕ | + | + | + | ⊕ |
| Sr | | ⊕ | | ⊕ | ⊕ | ⊕ | ⊕ | – | – | | ⊕ | | | © | ⊕ |
| Y | ⊕ | ⊕ | ⊕ | ⊕ | ⊕ | | – | | | | – | + | © | + | ⊘ |
| Zr | + | + | ⊕ | ⊕ | ⊕ | | | | | | – | + | + | | |
| Ba | + | ⊕ | + | ⊕ | ⊕ | ⊕ | ⊕ | + | ⊗ | ⊗ | ⊕ | + | ⊗ | + | ⊕ |
| La | + | ⊕ | ⊕ | ⊕ | ⊕ | ⊕ | ⊕ | ⊕ | © | © | ⊕ | + | © | ⊕ | ⊕ |
| Ce | ↔ | ⊕ | ⊕ | ⊕ | ⊕ | ⊕ | ⊕ | ⊕ | © | ⊕ | ⊕ | © | © | ⊕ | ⊕ |
| Pr | + | ⊕ | ⊕ | ⊕ | ⊕ | © | ⊕ | © | + | © | ⊕ | © | © | + | ⊕ |
| Nd | © | ⊕ | ⊕ | ⊕ | ⊕ | © | ⊕ | ⊕ | © | © | ⊕ | + | © | ⊕ | ⊕ |
| Pm | + | + | + | + | ⊕ | + | + | + | + | + | + | + | + | + | + |
| Sm | © | ⊕ | ⊕ | ⊕ | ⊕ | © | + | ⊕ | + | © | ⊕ | + | © | ⊗ | ⊕ |
| Eu | + | + | ⊕ | ⊕ | ⊕ | ⊕ | © | + | © | © | ⊕ | + | © | ⊕ | ⊕ |
| Gd | © | ⊕ | ⊕ | ⊕ | ⊕ | © | + | © | © | ⊕ | ⊕ | © | ⊕ | ⊕ | ⊕ |
| Tb | © | ⊕ | ⊕ | ⊕ | ⊕ | © | + | ⊕ | © | © | + | © | © | + | ⊕ |
| Dy | © | ⊕ | ⊕ | ⊕ | ⊕ | © | + | ⊕ | © | © | + | + | + | ⊕ | ⊕ |
| Ho | © | ⊕ | ⊕ | ⊕ | ⊕ | © | + | © | + | © | + | © | + | ⊗ | ⊕ |
| Er | © | ⊕ | ⊕ | ⊕ | ⊕ | © | + | ⊕ | © | © | + | © | © | ⊕ | ⊕ |
| Tm | © | © | ⊕ | ⊕ | ⊕ | © | + | © | + | © | + | + | + | ⊕ | + |
| Yb | © | ⊕ | ⊕ | ⊕ | ⊕ | © | + | ⊕ | ⊕ | ⊕ | ⊕ | + | + | ⊕ | ⊕ |
| Lu | © | © | ⊕ | ⊕ | ⊕ | © | + | © | © | © | + | + | + | ⊕ | + |
| Hf | + | + | ↔ | ⊕ | ⊕ | | | | | | | | | | |
| Ac | + | + | + | + | + | + | | + | + | + | + | + | + | + | + |
| Th | ⊕ | ⊕ | ⊕ | ⊕ | ⊕ | ⊕ | | © | © | © | + | © | © | © | © |
| Pa | + | + | | + | + | + | | + | + | + | + | + | + | + | + |
| U | © | © | | © | ⊕ | © | | © | © | © | + | © | ⊕ | © | © |
| Np | ⊕ | ⊕ | ⊕ | ⊕ | ⊕ | | | + | + | + | + | + | + | + | + |
| Pu | + | + | | + | + | + | | + | + | + | + | + | + | + | + |
| Am | + | + | | + | + | + | + | + | + | + | + | + | + | + | + |
| Cm | + | + | | + | + | + | | + | + | + | + | + | + | + | + |

**Notes**. The following notations are used: +, prediction of the $ThCr_2Si_2$ structural type for a compound with the composition $AB_2Si_2$; –, prediction of the absence of a compound with the composition $AB_2Si_2$ having the $ThCr_2Si_2$ structural type in the A – B – Si system; ⊕, a compound with the composition $AB_2Si_2$ has the $ThCr_2Si_2$ structural type and this fact was used for computer learning; ↔, in the A – B – Si system, no compound with the composition $AB_2Si_2$ was found or it exists, but has a structure different form that for $ThCr_2Si_2$, and this fact was used for computer learning; ©, prediction of the $ThCr_2Si_2$ structural type was confirmed experimentally; ⊗, prediction of the $ThCr_2Si_2$ structural type for a compound with the composition $AB_2Si_2$ was not confirmed experimentally; ⊘, prediction of the structural type different from $ThCr_2Si_2$, was not confirmed experimentally. Here and in other Tables the blank spaces correspond to the disagreement of the predictions with the use of different sets of the element properties; all data and predictions are given for the compounds under ambient conditions.

arsenic.[119–121] For the compounds with silicon and phosphorus, the structures of the ZrNiAl, PbFCl or TiNiSi type were predicted.[119,120] The prediction of the possibility of crystallization in the ZrNiAl structural type was performed for compounds with gallium and palladium.[119,121] The phases with the structures PbFCl and MgAgAs were predicted for the compounds with the composition ABSb.[120] The crystal structure of the MgAgAs type was predicted for equiatomic compounds with bismuth.[120]

The algorithm based on the training of the growing pyramidal networks was used in the search for the criteria of stability of crystal structures.[107] The formation of the stability criteria of certain crystal structures for each of the nine compositions (ABAl, ABSi *etc*.) was performed in two spaces of the element properties A and B considered in the previous section. The possibility of crystallization in one of several structural types was considered and the procedure of the consecutive dichotomy was used. For example, at the beginning the search for the criteria of the classification of chemical systems was performed, in which the phases with the ZrNiAl structural type are formed or not. Then the systems were classified according to the formation or the lack of formation of the equiatomic compounds of the TiNiSi structural type, *etc*.

Tables 5–7 contain examples of the predictions obtained by comparing the results for each pair of criteria of the crystal phase stability found in the computer training, which include one of the two sets of properties given above as parameters.

A comparison of the results of the prediction[121] with newer experimental data has shown that the prediction error for compounds ABAl is lower than 13%, for compounds ABIn it is $<22\%$, while for compounds ABBi all 22 predictions tested were in agreement with the experiment.[120] The mean prediction error of the crystal structure type of the equiatomic phases with the composition ABX (X = Al, Si, P, Ga, Ge, As, Pd, Sb, Bi) is equal to 34%.

**Table 3**. Examples of the predictions of compounds with the composition $AB_2Ge_2$ having the $ThCr_2Si_2$ structural type.[122]

| Element B | Element A: Cr | Mn | Fe | Co | Ni | Cu | Ru | Rh | Pd | Ag | Os | Ir | Pt | Au |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Ca | | | | | | ⊕ | | | + | ⊕ | | | | ⊕ |
| Sr | + | | | | | ⊕ | | | + | ⊕ | | | | ⊕ |
| Y | | ⊕ | | ⊕ | ⊕ | ⊕ | | | | − | | | | |
| Ba | + | | | | | + | + | + | + | ⊕ | | | + | |
| La | + | ⊕ | ⊕ | ⊕ | ⊕ | ⊕ | © | © | ⊕ | © | + | ⊗ | ⊕ | + |
| Ce | + | ⊕ | ⊕ | ⊕ | ⊕ | ⊕ | © | © | ⊕ | © | | | ⊕ | |
| Pr | + | ⊕ | ⊕ | ⊕ | ⊕ | ⊕ | © | © | + | © | | | ⊗ | |
| Nd | + | ⊕ | ⊕ | ⊕ | ⊕ | ⊕ | © | © | ⊕ | © | | | ⊕ | |
| Pm | + | + | | | | + | + | © | + | + | | | + | |
| Sm | + | ⊕ | | ⊕ | ⊕ | ⊕ | © | © | + | + | | | ⊗ | |
| Eu | + | © | | | ⊕ | © | © | © | © | © | | | ⊗ | |
| Gd | + | ⊕ | ⊕ | ⊕ | ⊕ | ⊕ | © | ⊕ | © | + | + | ⊗ | ⊕ | + |
| Tb | + | ⊕ | ⊕ | + | ⊕ | ⊕ | © | © | + | + | + | + | ⊗ | + |
| Dy | + | ⊕ | ⊕ | | ⊕ | ⊕ | © | © | ⊕ | + | | | ⊕ | |
| Ho | + | ⊕ | | ⊕ | ⊕ | ⊕ | © | © | © | + | | | + | |
| Er | + | ⊕ | ⊕ | ⊕ | ⊕ | ⊕ | © | © | + | + | | | + | |
| Tm | + | © | | ⊕ | ⊕ | ⊕ | © | © | + | + | | | + | |
| Yb | + | ⊕ | ⊕ | ⊕ | ⊕ | ⊕ | © | © | ⊕ | + | | | + | |
| Lu | + | © | + | ⊕ | ⊕ | + | © | + | + | + | + | + | + | + |
| Ra | | | | + | | + | | | | | | | | + |
| Ac | + | | + | + | + | + | + | + | | + | + | + | + | + |
| Th | ⊕ | ⊕ | ⊕ | ⊕ | ⊕ | ⊕ | © | ⊕ | ⊕ | + | © | © | ⊕ | ⊕ |
| Pa | + | | + | + | + | + | + | + | + | | + | + | + | + |
| U | ⊕ | ⊕ | ⊕ | ⊕ | ⊕ | ⊕ | + | ⊕ | ⊕ | | + | ⊕ | ⊕ | + |
| Np | + | | © | + | + | + | + | + | + | | + | + | + | + |
| Pu | + | | + | + | + | + | + | + | + | | + | + | + | + |
| Am | + | | + | + | + | + | + | + | + | | + | + | + | + |
| Cm | + | | + | + | + | + | + | + | + | | + | + | + | + |

**Notes**. The following notations are used: +, prediction of the $ThCr_2Si_2$ structural type for a compound with the composition $AB_2Ge_2$; −, prediction of the absence of a compound with the composition $AB_2Ge_2$ with the $ThCr_2Si_2$ structural type in the A–B–Ge system; ⊕, a compound with the composition $AB_2Ge_2$ has the structure of $ThCr_2Si_2$ type, and this fact was used for computer learning; ©, prediction of the $ThCr_2Si_2$ structural type was confirmed experimentally; ⊗, prediction of the $ThCr_2Si_2$ structural type for a compound with the composition $AB_2Ge_2$ was not confirmed experimentally.

## 3. The Heusler phases with the composition $ABX_2$

Substances possessing unique ferromagnetic properties, as well as giant magnetoresistance, magnetocaloric effect, high deformation, superplasticity and other properties, were found among compounds with the Heusler-type crystal structure.[136–140] In this connection, we have carried out design of the Heusler phases not yet synthesized with the compositions $ABX_2$ (X = Co, Ni, Cu, Pd) and $AB_2X$ (X = Al, Ga, In) possessing a cubic structure of the $MnCu_2Al$ type.[121, 124]

Using the ConFor[107] algorithm for each of the seven aforementioned compositions, the classification criteria were created that divide the chemical systems into two classes, *viz*., systems with the formation of a compound of the $ABX_2$ (or $AB_2X$) composition with the $MnCu_2Al$ structure and systems where such a compound is not formed under ambient conditions. The training sets were very small; they comprised less than 50 examples. For the description of the chemical properties, two sets of the properties of elements A and B as specified in Section IV.1 were used.

A comparison of the experimental results with the predictions made with the use of two sets of the element properties for the compositions $AB_2In$ and $ABCu_2$ are presented in Tables 8 and 9.

The test of 24 compositions $AB_2In$ has shown that four of them did not coincide with the experiment, *i.e*., the prediction error is 17%. For the compounds with the composition $ABCu_2$, 13 predictions have been tested experimentally. Only in one case, the calculations did not agree with the experimental results (the prediction error is 8%). The everage error of the prediction of the crystal structure type for the compounds with the compositions $ABX_2$ (X = Co, Ni, Cu, Pd) and $AB_2X$ (X = Al, Ga, In) is equal to 30%.

The advantage of computer design methods for the intermetallic compounds is the possibility of fast correction of the classification regularities with the appearance of new compounds for which the experimental information contradicts the obtained predictions. To this end, one should just add new examples to those previously used in the computer analysis and perform additional learning of the information-analytical system. Such an accommodation capability is a distinctive feature of the artificial intelligence methods the ideas of which underlie the computer system considered above for the design of inorganic compounds.[130] Taking

**Table 4**. Examples of prediction of the crystal structure type for compounds with the composition $AB_2P_2$.[120]

| Element A | Element B | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | Li | Be | Mg | Mn | Fe | Co | Ni | Cu | Zn | Ru | Rh | Pd | Cd |
| K | | | | | (T) | (T) | | T | T | (T) | (T) | | |
| Ca | C | (C) | | (C) | (T) | (T) | (T) | (T) | (C) | | | (T) | (C) |
| Sr | C | C | C | (C) | (T) | (T) | (T) | (T) | (C) | | | (T) | (C) |
| Y | C | | | | T | T | (T) | T | C | | | (T) | |
| Zr | C | C | C | C | | | | (C) | C | | | | |
| Cs | | | | | T | | | | | | | | |
| Ba | C | C | (C) | | (T) | (T) | (T) | (T) | (T) | | | (T) | (C) |
| La | (C) | | | | T© | (T) | (T) | T | T | T© | T¢ | (T) | |
| Ce | (C) | C | C | | T© | (T) | (T) | T | T | | | (T) | C |
| Pr | (C) | | | | T© | (T) | (T) | T | T | | | (T) | |
| Nd | (C) | | | | T | (T) | (T) | T | | | | (T) | |
| Pm | C | | | | T | T | T | T | | | | T | |
| Sm | C | C | C | | T | (T) | (T) | T | T | | | (T) | C |
| Eu | C | C | C© | (C) | T© | (T) | (T) | (T) | (C) | | | (T) | (C) |
| Gd | C | C | C | C | (T) | T | (T) | (T) | C | T© | T | (T) | C |
| Tb | (C) | C | C | | T | | (T) | T | T | | | (T) | C |
| Dy | C | C | C | | T | | (T) | T | TC | | | (T) | C |
| Ho | C | | | | T | | (T) | T | T | | | (T) | |
| Er | C | | | | T | | (T) | T | T | | | (T) | |
| Tm | C | | | | T | T | (T) | T | T | | | | |
| Yb | C | C | C© | C | T | | (T) | (C) | (C) | | | (T) | (C) |
| Lu | C | | | | T | T | T | | C | T© | T | T | |
| Ac | C | | | | | | | | C | | | | |
| Th | C | C | C | C | | | | (C) | C | | | | C |
| Pa | C | | | | | | | | C | | | | |
| U | C | | | | | | | | C | | | | |

**Notes**. The following notations are used: T, prediction of the $ThCr_2Si_2$ structural type for a compound with the composition $AB_2P_2$; C, prediction of the $CaAl_2Si_2$ structural type for a compound with the composition $AB_2P_2$; in parentheses, information on compounds used in computer learning; ©, prediction was confirmed experimentally; ¢, the prediction was not confirmed experimentally.

**Table 5**. Examples of the predictions of compounds with the composition ABAl with the TiNiSi structural type.[121]

| Element B | Element A | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | La | Ce | Pr | Nd | Pm | Sm | Eu | Gd | Tb | Dy | Ho | Er | Tm | Yb | Lu |
| Ru | – | O | – | – | – | + | – | + | + | + | + | + | + | – | – |
| Rh | – | O | ⊘ | ⊘ | – | + | – | © | + | + | © | + | © | ⊘ | – |
| Os | + | + | + | + | + | + | + | + | + | + | + | + | + | + | + |
| Ir | © | © | © | © | + | © | + | © | © | © | © | © | © | + | © |
| Pt | + | © | © | © | + | ⊕ | + | ⊕ | ⊕ | ⊕ | ⊕ | ⊕ | ⊕ | © | |

**Notes**. The following notations are used: +, prediction of the TiNiSi structural type for a compound with the composition ABAl; –, prediction of the absence of a compound with the composition ABAl with the TiNiSi structural type in the A–B–Al system; ⊕, a compound with the composition ABAl has the TiNiSi structural type, and this fact was used for computer learning; ©, prediction of the TiNiSi structural type was confirmed experimentally; O, prediction of a structure different from TiNiSi was confirmed experimentally; ⊘, the experiment did not confirm the prediction of the structure different from TiNiSi.

into account that the everage error value for the prediction of the Heusler phases is rather high (30%) and also that in the past years more than 100 new compounds with this structure were synthesized, it was decided to carry out computer learning with inclusion of newer data, with wider combination of properties of the elements and with a set of new programmes for pattern recognition.

The computer training set comprised information on 278 Heusler phases, 70 compounds with the $MgCuAl_2$ structure, 38 compounds with the $GdSnPt_2$ structure, 37 compounds with the $YSiPd_2$ structure, 20 compounds with the NaTl structure, 11 compounds with the $PrGaGo_2$ structure, 10 compounds with the $YSiRh_2$ structure, 16 compounds with the structures different from those listed above, as well as 486 examples where the compounds with the compositions $ABX_2$ (X = Mg, Al, Fe, Co, Ni, Cu, Ru, Rh, Pd, Ag, Ir, Pt or Au) were absent. This altogether

**Table 6**. Examples of the prediction of compounds with the composition ABIn with the ZrNiAl structural type.[121]

| Element B | Element A: Pr | Nd | Pm | Sm | Eu | Gd | Tb | Dy | Ho | Er | Tm | Yb | Lu | Pa | U |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Ni | ⊕ | ⊕ | + | ⊕ | | ⊕ | ⊕ | ⊕ | ⊕ | ⊕ | ⊕ | | © | + | |
| Ru | + | + | + | + | + | + | + | + | + | + | + | + | + | + | © |
| Rh | © | ⊕ | + | © | ⊗ | ⊕ | © | ⊕ | © | ⊕ | © | ⊗ | ⊗ | + | + |
| Pd | ⊕ | ⊕ | | ⊕ | ⊕ | ⊕ | ⊕ | ⊕ | ⊕ | ⊕ | ⊕ | ⊕ | ⊕ | + | © |
| Ag | + | + | + | + | + | + | + | + | + | + | + | + | + | + | + |
| Os | + | + | + | + | + | + | + | + | + | + | + | + | + | + | + |
| Ir | + | + | + | © | + | © | © | © | © | + | + | + | + | + | + |
| Pt | © | ⊕ | + | © | ⊗ | ⊕ | © | ⊕ | © | ⊕ | ⊕ | © | ⊕ | + | ⊕ |
| Au | ⊕ | ⊕ | + | ⊕ | ⊗ | ⊕ | ⊕ | ⊕ | ⊕ | ⊕ | + | ⊕ | + | + | + |

**Notes**. The following notations are used: +, prediction of the ZrNiAl structural type for a compound with the composition ABIn; ⊕, a compound with the composition ABIn has the structure of the ZrNiAl type, and this fact was used in computer learning; ©, prediction of the ZrNiAl structural type for a compound with the composition ABIn was confirmed experimentally; ⊗, the experiment did not confirm the prediction of the ZrNiAl structural type for a compound with the composition ABIn.

**Table 7**. Examples of predictions of compounds with the composition ABBi having the MgAgAs structural type.[120]

| Element B | Element A: Ca | Ni | Pd | Pt | Element B | Element A: Ca | Ni | Pd | Pt |
|---|---|---|---|---|---|---|---|---|---|
| Ni | + | | | | Gd | | ⊕ | ⊕ | ⊕ |
| Ba | + | + | | | Tb | | © | © | © |
| La | | + | © | © | Dy | | ⊕ | ⊕ | ⊕ |
| Ce | | + | ⊕ | ⊕ | Ho | | © | ⊕ | ⊕ |
| Pr | | © | © | © | Er | | © | © | ⊕ |
| Nd | | © | © | © | Tm | | ⊕ | © | © |
| Pm | | + | + | + | Yb | | + | ⊕ | ⊕ |
| Sm | | © | © | © | Lu | | © | © | © |
| Eu | | + | + | + | | | | | |

**Notes**. The following notations are used: +, prediction of the MgAgAs structural type for a compound with the composition ABBi; ⊕, a compound with the composition ABBi has the MgAgAs structural type, and this fact was used in computer learning; ©, the prediction of the MgAgAs structural type was confirmed experimentally.

was extracted from the database 'Phases' on the properties of inorganic compounds (http://phases.imet-db.ru).[58]

Information on the metallic systems was represented in the computer memory as a set of values of properties of chemical elements A, B and X, such as the pseudo-potential radii (according to Zunger), melting, boiling and the Debye temperatures, first three ionization potentials, the distances to core and valence electrons (according to Schubert), the regular numbers (according to Mendeleev–Pettifor), electronegativities (according to Pauling), the Miedema chemical potentials, the quantum numbers, thermal conductivities, the Group number in the Periodic system, molar heat capacities, melting, evaporation and atomization enthalpies, entropies of the solid state, the atomic masses, densities, the linear coefficients of thermal expansion, the metallic radii (according to Waber), *etc*., 108 values in total for each system. The data on the properties of the elements were taken from the database 'Elements' (http://phases.imet-db.ru/elements).

**Table 8**. Examples of predictions of the Heusler phases with the composition $AB_2In$.[121]

| Element B | Element A: Ru | Rh | Pd | Ag | Os | Ir | Pt | Au |
|---|---|---|---|---|---|---|---|---|
| Ti | | | ⊕ | + | | | ⊕ | ⊕ |
| Sr | | | | + | | | | |
| Y | | | ⊕ | © | | | | ⊕ |
| Zr | + | + | ⊕ | + | + | + | ⊕ | ⊕ |
| Nb | + | + | + | + | + | + | + | + |
| Tc | + | + | + | + | + | + | + | + |
| La | + | + | ⊗ | © | + | + | + | ⊕ |
| Ce | | | | © | | | | |
| Pr | + | + | + | © | + | + | + | ⊕ |
| Nd | + | + | + | © | + | + | + | ⊕ |
| Pm | + | + | + | + | + | + | + | + |
| Sm | + | + | + | © | + | + | + | ⊕ |
| Eu | + | + | + | + | + | + | + | + |
| Gd | + | + | © | © | + | + | ⊗ | © |
| Tb | + | + | + | © | + | + | ⊗ | ⊕ |
| Dy | + | + | © | © | + | + | + | ⊕ |
| Ho | + | + | + | © | + | + | ⊗ | ⊕ |
| Er | + | + | © | © | + | + | + | ⊕ |
| Tm | + | + | © | © | + | + | + | © |
| Yb | + | + | + | + | + | + | + | ⊕ |
| Lu | + | + | © | + | + | + | + | © |
| Hf | + | + | ⊕ | + | + | + | ⊕ | ⊕ |
| Ta | | | | + | | | | |
| Re | − | | | + | | | | |

**Notes**. The following notations are used: +, predictions of the $MnCu_2Al$ structural type for a compound with the composition $AB_2In$; −, prediction of the absence of a compound with the composition $AB_2In$ with the $MnCu_2Al$ structural type; ⊕, a compound with the composition $AB_2In$ has the $MnCu_2Al$ structural type, and this fact was used in computer learning; ©, prediction of the formation of a compound with the composition $AB_2In$ and the $MnCu_2Al$ structural type was confirmed experimentally.

**Table 9**. Examples of the prediction of the Heusler phases with the composition $ABCu_2$.[124]

| Element B | Element A: Li | Be | Al | K | Sc | V | Cr | Fe | Co | Ni | Ga | Ge | Y | Nb | Mo | Ru | Rh | Pd | Ag | In |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Zn | | | © | | | | | | | | | – | – | – | – | – | – | – | O | |
| Ga | + | + | | + | ⊕ | + | + | + | + | + | | O | | | | | | | – | + |
| In | + | + | | + | © | + | + | + | + | + | + | + | © | + | + | + | + | + | ⊗ | |
| Sn | O | – | O | – | – | – | | ⊕ | ⊕ | ⊕ | – | – | – | ↔ | – | – | – | – | ↔ | © |
| Lu | – | – | | – | – | – | – | – | – | – | | – | – | – | – | – | – | – | – | © |
| Ta | | – | | | – | – | – | – | – | ↔ | | – | – | ↔ | – | – | – | – | | + |
| Au | – | – | | – | – | – | – | – | – | O | | – | – | – | – | – | – | ↔ | ↔ | + |
| Tl | | | | | | | | | | | | – | | | | | | | – | + |
| Pb | – | – | O | – | – | – | – | – | – | – | – | – | – | – | – | – | – | – | O | + |

**Notes**. The following notations are used: +, prediction of the $MnCu_2Al$ structural type for a compound with the composition $ABCu_2$; –, prediction of the absence of a compound with the composition $ABCu_2$ and the $MnCu_2Al$ structural type; ⊕, compound with the composition $AB_2Cu$ has the $MnCu_2Al$ structural type, and this was used in computer learning; ↔, no compound with the composition $AB_2Cu$ was found in the A–B–Cu system or it exists, but has a structure different from that of $MnCu_2Al$, and this fact was used in computer learning; ©, prediction of the formation of a compound with the composition $ABCu_2$ and the $MnCu_2Al$ structural type was confirmed experimentally; O, prediction of a compound with the composition $ABCu_2$ and the structure different from $MnCu_2Al$ was confirmed experimentally.

For computer learning, the following algorithms and methods were used that underlie the pattern recognition programmes constituting the information-analytical system: the estimate calculation algorithm,[94, 131] linear machine, Fisher's linear discriminant, logical regularities, multi-level perceptron (method of the inverse error distribution), *k*-nearest neighbours,[131, 141] support vector machine,[127, 131] statistical vector syndromes,[131, 142] method of binary decision trees,[98] method of two-dimensional linear separators,[143] the system of concept formation ConFor based on the usage of the growing pyramidal networks.[107]

The procedure of computer design of the intermetallic compounds included three stages:

— prediction of the chemical systems A–B–X with and without formation of compounds with the composition $ABX_2$;

— multiclass prediction of the crystal structure type: the Heusler phases, compounds with structures of the NaTl, $YSiRh_2$, $MgCuAl_2$, $GdSnPt_2$, $YSiPd_2$, $PrGaCo_2$ types, compounds with the structures different from those listed above and the lack of compounds with the composition $ABX_2$ (9 classes in total);

— consecutive partitioning of systems in three classes, for example, the Heusler phases, compounds with the structures different from the structure of the Heusler phases, the absence of compounds with the composition $ABX_2$ in the A–B–X system.

At any stage, each programme for pattern recognition created the classifying regularity where the properties of chemical elements, the components of the chemical systems A–B–X, serve as the variables. For the selection of the most accurate programme for the prediction of compounds not yet synthesized, we used the procedure of cross-validation. Here, a definite part of objects (*f*), descriptions of the A–B–X systems, are withdrawn from the training set, and then the computer learning is performed with the remaining objects, while the withdrawn objects are used for the exam recognition. The number of errors is recorded. Then the 'control' objects are returned to the training set and the next *f* objects are withdrawn. This procedure is repeated until all objects of the training set have served as the control objects. This allows a more unbiased estimation of the precision of computer learning algorithms for a given training set and for the application of pattern recognition methods to avoid the undesirable procedure of 'overfitting' (see above).

Upon completion of learning with the cross-validation, the everage error for the exam recognition is evaluated, which is later used for the selection of the best algorithms in making the collective decision.

The goal of the application of the strategy of collective decisions is the increase in the prediction accuracy. The idea of this approach is as follows. First, different algorithms of computer learning are successively used for the prediction of new compounds. Then the results of each separate algorithm are specially processed [131] and the final collective decision on the assignment of particular compounds to a certain class is made. More often the use of such 'collective intelligence' allows compensating the prediction errors obtained with the application of separate algorithms, and in the majority of cases one can obtain a more accurate result.

The simplest collective method is the voting of predictions in which a result most often predicted by different algorithms is chosen. However the voting of predictions does not always allow enhancing the accuracy of the predictions, especially in the cases of the inadequate fulfilment of the main hypothesis of pattern recognition, *i.e.*, hypothesis of the object compactness in the feature space.[131] More sophisticated algorithms of collective decision making such as the Woods dynamic method, the Bayesian methods, logical correction of the set of the recognition algorithms, clustering and selection decision templates, *etc.*[131] are designed for solving very complicated problems of predictions.

The best algorithm of collective decision making was chosen based on the results of recognition of 100 objects, their numbers were taken from the table of random numbers (uniform distribution) and they were withdrawn from the training set during learning and collective decision-making processes. In the last stage of the design of compounds, the objects used for the estimation of the recognition quality were added to the training set and the process

**Table 10**. The accuracy of the examination recognition (%) with cross-validation in the prediction of the possibility of formation and crystal structure type for the intermetallics with the composition $ABX_2$.

| Algorithm | Possibility of formation of the compound | Multiclass prediction | Predicted class (successive separation) | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| | | | the Heusler phases | NaTl | $YSiRh_2$ | $MgCuAl_2$ | $GdSnPt_2$ | $YSiPd_2$ | $PrGaCo_2$ |
| Estimates calculation algorithm | 80.0 | 60.4 | 71.9 | 81.6 | 79.5 | 67.6 | — | 53.9 | 58.0 |
| Two-dimensional linear separators | 80.0 | — | 71.6 | 81.3 | 74.2 | 42.7 | 37.2 | 51.1 | 49.1 |
| Binary decision trees | 56.9 | 63.1 | 47.5 | 50.6 | 53.2 | 57.7 | 40.8 | 40.7 | 48.4 |
| Fisher's linear discriminant | 81.3 | 76.5 | 70.6 | 80.9 | 79.3 | *65.2* | 58.9 | *62.9* | *66.5* |
| *Linear machine* | *88.0* | *84.1* | *83.8* | *86.6* | *87.5* | 58.9 | 44.7 | *59.9* | *61.8* |
| *Logical regularities* | *86.0* | *76.8* | *82.6* | *86.9* | *85.4* | *64.3* | *52.0* | *57.3* | *60.2* |
| Neural networks | 82.9 | 68.5 | 70.2 | 79.3 | 82.2 | — | — | — | 56.7 |
| *k-Nearest neighbours* | *92.3* | *89.6* | *89.4* | *93.5* | *94.1* | *63.4* | *44.7* | 40.7 | 39.7 |
| Support vectors machine | *59.3* | 59.0 | 60.2 | 73.7 | 94.5 | 48.0 | 51.2 | 49.5 | 54.7 |
| Statistically weighted syndromes | — | 28.8 | 75.2 | — | 76.9 | — | 20.6 | 43.2 | 45.4 |
| *ConFor* | *97.0* | *95.2* | *91.3* | *91.8* | *90.0* | *86.7* | *82.4* | *81.4* | *83.5* |

**Table 11**. The accuracy of the examination recognition (%) with cross-validation using different procedures of making the collective decision in the prediction of the possibility of the formation and of the crystal structure type for intermetallics with the composition $ABX_2$.

| Algorithm | Possibility of formation of the compound | Multiclass prediction | Predicted class (successive separation) | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| | | | the Heusler phases | NaTl | $YSiRh_2$ | $MgCuAl_2$ | $GdSnPt_2$ | $YSiPd_2$ | $PrGaCo_2$ |
| The Bayesian method | *100.0* | 99.2 | 99.7 | 100.0 | 98.6 | 94.7 | 92.1 | *97.0* | 96.5 |
| Clustering and selection | 100.0 | 100.0 | 100.0 | 100.0 | 96.2 | 94.5 | 91.3 | 93.4 | 93.8 |
| Decision templates | 100.0 | 100.0 | 100.0 | 100.0 | *98.8* | 96.8 | 93.9 | 96.4 | *96.6* |
| The Woods dynamic method | 77.9 | 76.2 | 98.9 | 81.2 | 86.7 | 87.1 | 94.4 | 81.4 | 79.7 |
| The complex committee method (voting on the majority) | 96.5 | 92.3 | 95.8 | 97.4 | 97.2 | 86.3 | 62.5 | 92.4 | 92.5 |
| *The complex committee method (averaging)* | 96.5 | *100.0* | *100.0* | *100.0* | 98.6 | *96.9* | 95.1 | 94.7 | 95.1 |
| Logical correction | — | 99.8 | 99.9 | 100.0 | 98.7 | 90.6 | *95.6* | 92.1 | 92.2 |

of the collective decision making was re-initiated using the pre-chosen best algorithm. The most 'accurate' learning and collective decision-making algorithms were used for the prediction. The assignment of a not yet studied chemical system to a certain pre-determined class was predicted by inserting only the values of properties of the elements that components of this system into the found regularities. The final result of the prediction was formed based on the comparison of the results of prediction in all three stages.

The results of the exam recognition with cross-validation are given in Table 10. The best algorithms (italisized) were used in making the collective decision, which is given in Table 11 (the method that was later applied for the prediction of new compounds is italisized). It should be noted that the accuracy of the prediction became significantly higher with the use of a 'collective of algorithms'.

Part of the results of the prediction of the crystal structure type for the intermetallic compounds with the compositions $ABRu_2$, $ABRh_2$ and $ABPd_2$ is given in Tables 12–14.

Predictions of the Heusler phases with noble metals are of particular interest in the search for new magnetic nanomaterials. The thing is that the Heusler alloys based on cobalt, iron or nickel have recently found applications for the production of the computer hard disks. The use of nanopowders of the Heusler phases was suggested in order to increase the information density on the disks. One of the problems in this case, however, is especially high reactivity of the cobalt, iron or nickel nanopowders. Therefore, an experimental search for new, more chemically stable ferromagnetic Heusler phases with noble metals was begun. The results obtained will allow reduction of time and costs for the search of such compounds.

**Table 12**. Prediction of the crystal structure type for compounds with the composition $ABRu_2$.

| Element B | Element A: Li | Be | Mg | Al | Si | Sc | Ti | V | Cr | Mn | Fe | Co | Ni | Cu | Zn | Ga | Ge | Y | Zr | Nb | Pd | Ag | In | Sn | Sb | Hf | Ta | Tl |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Mg | | 9 | | | | | | | | | | | | | | | | | | | | | | | | | | |
| Si | 1 | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| V | | | 9 | | | | 9 | | | | | | | | | | | | | | | | | | | | | |
| Cr | | | 9 | | | | 9 | 9 | | | | | | | | | | | | | | | | | | | | |
| Mn | | | | 1 | #1 | 9 | 9 | 9 | 9 | | | | | | | | | | | | | | | | | | | |
| Fe | | 9 | 9 | | #1 | | 9 | 9 | 9 | 9 | | | | | | | | | | | | | | | | | | |
| Co | 9 | 9 | 9 | 9 | 9 | 9 | 9 | 9 | 9 | 9 | #9 | | | | | | | | | | | | | | | | | |
| Ni | 9 | 9 | 9 | #9 | | 3 | #9 | 9 | 9 | 9 | 9 | 9 | | | | | | | | | | | | | | | | |
| Cu | | 9 | | | | | 9 | 9 | 9 | 9 | 9 | 9 | 9 | | | | | | | | | | | | | | | |
| Zn | | 9 | | | | | 9 | 9 | 9 | 9 | 9 | 9 | 9 | 9 | | | | | | | | | | | | | | |
| Ga | | | | | | | 1 | 1 | | 1 | | | 9 | | | | | | | | | | | | | | | |
| Ge | 1 | | | | | | | | | #1 | | | 9 | 9 | 9 | | | | | | | | | | | | | |
| Y | | | | | 3 | | | 5 | 3 | | | 9 | | | | | 3 | | | | | | | | | | | |
| Zr | | | | | | | | 9 | 9 | | 9 | 9 | 9 | 9 | | | | | | | | | | | | | | |
| Nb | | | | | 9 | 9 | #9 | | 9 | 9 | 9 | 9 | 9 | 9 | 9 | | 9 | | #9 | | | | | | | | | |
| Pd | | 9 | 9 | | 9 | | 9 | 9 | 9 | 9 | 9 | 9 | 9 | 9 | 9 | | 9 | | | 9 | | | | | | | | |
| Ag | | 9 | | | 9 | | | 9 | 9 | 9 | 9 | 9 | 9 | 9 | 9 | | | | 9 | 9 | #9 | | | | | | | |
| In | | | | | 9 | | | | | 1 | 9 | 9 | 9 | 9 | | | | | | | | | | | | | | |
| Sn | | | 9 | 9 | | | | | | #1 | | | | | 9 | | | | | 9 | 9 | | | | | | | |
| Sb | | | | | | | | | | #1 | 9 | 9 | | 9 | 9 | 9 | | 3 | | 9 | 9 | | | | | | | |
| La | | | 3 | | 3 | | | | | | 9 | 9 | | 3 | | | | | | | | | | | 3 | | | |
| Ce | | | | | | | | | | | 9 | | | | | | | | | 7 | | 3 | | | | | | |
| Pr | | | | | 3 | | 7 | 7 | | | | | | 3 | | | 3 | | | | | | | | | | | |
| Nd | | | | | 3 | | | 7 | | | | | | 3 | 3 | | 3 | | | 7 | | 3 | | | | | | |
| Pm | | | | | 3 | | | 7 | | | 9 | | | | 3 | | 3 | | | 7 | | | | | 3 | | | |
| Sm | | 3 | | | 3 | | 7 | 7 | | | | | | | | | 3 | | | | 3 | 3 | | | | | | |
| Eu | | | | | 3 | | 7 | 7 | | | | | | | 3 | | 3 | | | | 3 | | | | | | | |
| Gd | | | | | 3 | | | | | | 9 | | | | | | 3 | | | | | | | | | | | |
| Tb | | | | | 3 | | | 7 | | | 9 | 9 | | 3 | | | | | | | 3 | | | | | | | |
| Dy | | | | | 3 | | | | | | 9 | | | 3 | | | | | | | | | | | | | | |
| Ho | | | | | 3 | | | | | | | | | 3 | | | | | | | | | | | | | | |
| Er | | | | | 3 | | | | | | | | | 3 | | | | | | | | | | | | | | |
| Tm | | | | | 3 | | | | | | | | | 3 | | 5 | | | | 8 | | | | | | | | |
| Yb | | | | | 3 | | | | | | | | | 3 | | 5 | | | | | | | | | | | | |
| Lu | | | | | 3 | | 7 | | | | | | | 3 | | | | | | | 9 | | | | | | | |
| Hf | | | | | | | 9 | 9 | 9 | 9 | 9 | 9 | 9 | 9 | 9 | | | | | #9 | 9 | 9 | | 1 | 9 | | | |
| Ta | | | 9 | | | | 9 | 9 | 9 | 9 | 9 | 9 | 9 | 9 | 9 | | | | 9 | #9 | 9 | 9 | | | 9 | 9 | | |
| Pt | | 9 | 9 | | 9 | 9 | 9 | 9 | #9 | 9 | 9 | 9 | 9 | 9 | 9 | | 9 | | 9 | 9 | 9 | 9 | | | 9 | 9 | 9 | |
| Tl | | | | | 9 | | | | 9 | | 9 | 9 | 9 | 9 | | | | | | | | | | | | 1 | | |
| Pb | | | 9 | 9 | | | | | | | 9 | 9 | | | | | | | | 9 | 9 | | | 9 | | | 9 | |
| Bi | | 9 | | 9 | | | | 9 | | | 9 | 9 | | | | | 9 | | | | 9 | | | 9 | | | 9 | 9 |
| Th | | | | | | | | | | | 9 | 9 | | 3 | | | | | | | | | | | | | | |
| U | | | | | | | | | | | 9 | | | | | | | | | | | | | | | | 9 | |

**Notes**. The following notations are used: 1, prediction of compounds $ABRu_2$ with the Heusler-type crystal structure; 3, prediction of a compound $ABRu_2$ with the $YSiRh_2$ structure; 5, prediction of a compound $ABRu_2$ with the $GdSnPt_2$ structure; 7, prediction of a compound $ABRu_2$ with the $PrGaCo_2$ structure; 8, prediction of a compound $ABRu_2$ with the structure different from those given above; 9, prediction of the absence of a compound with the composition $ABRu_2$. Here and in Tables 13, 14, # stands for the designation of systems that have been used in computer learning.

**Table 13**. Prediction of the crystal structure type for compounds with the composition $ABRh_2$.

| Element B | Element A | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | Li | Be | Mg | Al | Si | Sc | Ti | V | Cr | Mn | Fe | Co | Ni | Cu | Zn | Ga | Ge | Y | Zr | Nb | Ru | Pd | Ag | In | Sn | Sb | Pm | Eu | Gd | Er | Tm | Yb | Lu | Hf | Ta | Pt | Pb |
| Sc | 1 | 1 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| Ti | 1 | | | 1 | 1 | 1 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| V | 1 | | | 1 | 1 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| Mn | 1 | | | #1 | | 1 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| Ga | | | | | | 1 | 1 | 1 | | 1 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| Ge | #1 | | | | | | | | | 1 | | | 1 | | | | | | | | | | | | | | | | | | | | | | | | | |
| Y | | | | | #3 | 3 | | | 3 | | | | | 3 | | | #3 | | | | | | | | | | | | | | | | | | | | | | |
| Zr | | | | 1 | | | | | | | 9 | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| Nb | | | | 1 | | | | | 9 | | 9 | 9 | 9 | | | | | | | | | | | | | | | | | | | | | | | | | |
| Ru | | 9 | 9 | 9 | | #9 | 9 | 9 | 9 | 9 | 9 | 9 | 9 | 9 | 9 | 9 | | 9 | 9 | 9 | | | | | | | | | | | | | | | | | |
| Pd | | | 9 | 9 | 9 | 9 | | 9 | 9 | 9 | 9 | 9 | 9 | 9 | 9 | | 9 | | | 9 | 9 | | | | | | | | | | | | | | | | | |
| Ag | | | 9 | | 9 | | 9 | 9 | 9 | 9 | 9 | 9 | 9 | 9 | 9 | | | | 9 | 9 | 9 | #9 | | | | | | | | | | | | | | | | |
| In | | | | | | | 1 | 1 | 1 | | 9 | 9 | 9 | | | | | | 1 | 1 | | | | | | | | | | | | | | | | | | |
| Sn | | | | | | | | | | 1 | | 9 | 9 | | 9 | | | | | | 9 | 9 | 9 | | | | | | | | | | | | | | | |
| Sb | | | | 9 | | | | | | | 9 | 9 | | 9 | 9 | | | | | | 9 | | | 9 | 9 | | | | | | | | | | | | | |
| La | | | | | 3 | | | | | | | | | | | 5 | 3 | | | | | | | | | 3 | | | | | | | | | | | | |
| Ce | | | | | | | | | | | | 9 | | | | | 3 | | | | | | | | | 3 | | | | | | | | | | | | |
| Pr | | | | | 3 | | 3 | | 3 | | | | | | | | 3 | | | | | | | | | 3 | | | | | | | | | | | | |
| Nd | | | | | 3 | | | | 3 | | | | | | | | 3 | | | | | | | | | 3 | | | | | | | | | | | | |
| Pm | | | | | 3 | | | | | | | | | | | | 3 | | | | | | | | | 3 | | | | | | | | | | | | |
| Sm | | | | | 3 | | | | | | | | | | | | #3 | | | | | | | | | 3 | | | | | | | | | | | | |
| Eu | | | | | 3 | | | | | | | | | | | | 3 | | | | | | | | | 3 | | | | | | | | | | | | |
| Gd | | | | | 3 | | | | 3 | | | | | | | | 3 | | | | | | | | | | | | | | | | | | | | | |
| Tb | | | | | 3 | | | | | | | | | | | | 3 | | | | | | | | | 3 | | | | | | | | | | | | |
| Dy | | | | | 3 | | | | | | | | | | | 5 | 3 | | | | | | | | | 3 | | | | | | | | | | | | |
| Ho | | | | | 3 | | | | | | | | | | | 5 | 3 | | | | | | | | | 3 | | | | | | | | | | | | |
| Er | | | | | #3 | | | | | | | | | | | 5 | #3 | | | | | | | | | | | | | | | | | | | | | |
| Tm | | | | | 3 | 3 | | | | | | | | | | 5 | 3 | | | | | | | | | | | | | | | | | | | | | |
| Yb | | | | | 3 | | | 1 | | | | | | | | #5 | 3 | | 8 | | | | | | | | | | | | | | | | | | | |
| Lu | | | | | | 3 | | 8 | | | | | | | | | 3 | | 8 | | 9 | | | | | | | | | | | | | | | | | |
| Hf | | | | | | | | | | | 9 | | 9 | | | | | | | | 9 | 9 | | 1 | | | 8 | 8 | 8 | 8 | 8 | 8 | 8 | | | | |
| Ta | | | | | | | 9 | 9 | 9 | 9 | 9 | 9 | 9 | 9 | 9 | | | | 9 | 9 | 9 | 9 | 9 | 8 | | | | | | | | | | | | | |
| Pt | | 9 | 9 | | | | 9 | 9 | 9 | 9 | 9 | 9 | 9 | 9 | 9 | | 9 | | 9 | 9 | 9 | 9 | 9 | 9 | | 9 | | | | | | | | | 9 | 9 | | |
| Tl | | | | | | 1 | 1 | | | 1 | 9 | 9 | | | | | | | 1 | | 9 | | | | | | | | | | | | | | 1 | | | |
| Pb | | | | | | | | | | 1 | 9 | 9 | 9 | | | | | | | | 9 | | 9 | | 9 | | | | | | | | | | 1 | | | |
| Bi | | | | | | | | | 9 | | 9 | 9 | | | | | | | | | 9 | | 9 | | 9 | | | | | | | | | | | 9 | 9 | |
| U | | | | | 3 | | | | | | | | | | | | | | | | 9 | | | | | 3 | | | | | | | | | | | |

**Notes**. The following notations are used: 1, prediction of the $ABRh_2$ compounds with the Heusler-type crystal structure; 3, prediction of a compound $ABRh_2$ with the $YSiRh_2$ structure; 7, prediction of a compound $ABRh_2$ with the $PrGaCo_2$ structure; 8, prediction of a compound $ABRh_2$ with the structure different from those given above; 9, prediction of the absence of a compound with the composition $ABRh_2$.

**Table 14**. Prediction of the type of crystal structure for compounds with the composition $ABPd_2$.

| Element B | Element A: Li | Be | Mg | Al | Si | Sc | Ti | V | Cr | Mn | Fe | Co | Ni | Cu | Zn | Ga | Ge | Y | Zr | Nb | Ru | Ag | In | Sn | Sb | La | Ce | Pr | Nd | Pm | Sm | Eu | Gd | Tb | Dy | Ho | Er | Tm | Yb | Lu | Hf | Ta | Pt | Tl | Pb | Bi |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Al | 1 | | 1 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| Sc | 1 | | | #1 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| Ti | 1 | | | #1 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| V | 1 | | | 1 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| Cr | | | | 1 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| Mn | 1 | | | #1 | 1 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| Ga | | | 1 | | | #1 | 1 | 1 | | 1 | | | | 8 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| Zr | 1 | | | #1 | 6 | | | | | | | | | | 1 | 1 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| Nb | | | | 1 | | | | | | | | | | | 9 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| Ru | | | 9 | | 1 | | | | | 9 | 9 | 9 | 9 | 9 | 9 | | | 6 | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| Ag | | | 9 | #9 | #9 | | | | #9 | 9 | 9 | #9 | #9 | #9 | 9 | 9 | 9 | | | | #9 | | | | | | | | | | | | | | | | | | | | | | | | | |
| In | | | 1 | | | #1 | #1 | 1 | 1 | #1 | | | | | | 1 | | #1 | #1 | 1 | | | | | | | | | | | | | | | | | | | | | | | | | | |
| Sn | | | | | 9 | #1 | 1 | 1 | | #1 | | | | | 9 | | 9 | #1 | 1 | 1 | | 9 | #9 | | | | | | | | | | | | | | | | | | | | | | | | |
| Sb | | 1 | | | | 1 | 1 | 1 | | #1 | | | | 9 | | | | #1 | | | | 9 | | | | | | | | | | | | | | | | | | | | | | | | |
| La | | | | | 6 | | | | 6 | | | 6 | 6 | 6 | 6 | 6 | #6 | | | | 6 | | #5 | | 1 | | | | | | | | | | | | | | | | | | | | |
| Ce | | 6 | | 6 | #6 | | | 6 | 6 | | 6 | 6 | 6 | 6 | 6 | #6 | #6 | 6 | | 6 | 6 | | #5 | 6 | | 6 | | | | | | | | | | | | | | | | | | |
| Pr | | | | | #6 | | | | | | | | 6 | 6 | | | #6 | 6 | | | | | 1 | | | 6 | 6 | | | | | | | | | | | | | | | | | | |
| Nd | | | | | #6 | | | | | | | | 6 | 6 | | 6 | #6 | | | | | | 1 | | 1 | 6 | | 6 | | | | | | | | | | | | | | | | |
| Pm | | | | | 6 | | | | | | | | 6 | 6 | | | 6 | | | | | 6 | | 1 | 1 | 6 | 6 | | | | | | | | | | | | | | | | | | |
| Sm | | | | | #6 | | | | | | | | 6 | 6 | | 1 | #6 | | | | | | 1 | 1 | 1 | | | | | | | | | | | | | | | | | | | | |
| Eu | | | | | 6 | | | | | | | | 6 | 6 | | | #6 | | | | | | 1 | 1 | 1 | | 6 | | | | | | | | | | | | | | | | | | |
| Gd | | | | | #6 | | | | | 1 | | | 6 | 6 | | | #6 | | | | | | #1 | 1 | #1 | | | | | | | | | | | | | | | | | | | | |
| Tb | | | | | #6 | | | | | 1 | | | 6 | 6 | | | #6 | | | | | | 1 | #1 | 1 | 6 | 6 | | | | | | | | | | | | | | | | | | |
| Dy | | | | | #6 | | | | | 1 | | | 6 | 6 | | | #6 | | | | | | #1 | #1 | #1 | | 6 | | | | | | | | | | | | | | | | | | |
| Ho | | | | | #6 | | | | | 1 | | | 6 | 6 | | | #6 | | | | | | 1 | #1 | #1 | | 6 | | | | | | | | | | | | | | | | | | |
| Er | | | | | #6 | | | | | 1 | | | 6 | 6 | | | #6 | | | | | | #1 | #1 | #1 | | | | | | | | | | | | | | | | | | | | |
| Tm | | | | | #6 | | | | | | | | 6 | 6 | | | #6 | | | | | | #1 | #1 | 1 | | | | | | | | | | | | | | | | | | | | |
| Yb | | | | 1 | 6 | | 1 | | | 1 | | | | 6 | | | 6 | | | | | 6 | 1 | #1 | #1 | | | | | | | | | | | | | | | | | | | | |
| Lu | | | | | #6 | | | | | | | | 6 | 6 | | | #6 | | | | | | #1 | #1 | 1 | | 6 | | | | | | | | | | | | | | | | | | |
| Hf | 1 | | | #1 | | | | | | | | | | | 1 | 1 | | | | | | | #1 | 1 | | | | | | | | | | | | | | | | | | | | |
| Ta | 1 | | | | 6 | | | | | | | 9 | 9 | 9 | | | 6 | | | | | 9 | 1 | 1 | | | | | | | | | | | | | | | | | | 9 | | | | |
| Pt | | | 9 | 9 | | | | | 9 | 9 | 9 | 9 | #9 | 9 | 9 | 9 | | 6 | | 9 | 9 | #9 | 9 | 9 | 9 | 6 | 6 | 6 | 6 | 6 | 6 | 6 | 6 | 6 | 6 | 6 | 6 | 6 | 6 | 6 | 6 | | 9 | | | | |
| Tl | #8 | 1 | 1 | 1 | | 1 | 1 | 1 | 1 | 1 | | | | | | 1 | | #1 | 1 | 1 | | | | | | 1 | | 1 | 1 | #1 | 1 | #1 | 1 | #1 | #1 | #1 | 1 | 1 | 1 | 1 | 1 | | | | | |
| Pb | | | | | | 1 | | | | 1 | | | 9 | 9 | 9 | | | #1 | 1 | | | 9 | 9 | #9 | | 1 | 1 | #1 | 1 | 1 | #1 | 1 | #1 | #1 | #1 | #1 | #1 | 1 | #1 | 1 | 1 | | 9 | | | | |
| Bi | 1 | | | | 9 | 1 | 1 | 1 | | 1 | | | | 9 | 9 | | 9 | #1 | | | | 9 | 9 | 9 | 9 | 1 | 1 | #1 | 1 | 1 | #1 | 1 | #1 | #1 | #1 | #1 | #1 | 1 | #1 | 1 | 1 | | 9 | | | | |
| Th | | | | | 6 | | | | | | | | 6 | 6 | | | 6 | | | | | 6 | | 1 | 1 | 6 | 6 | 6 | | | | | | | | | | | | | | | | 1 | 1 | 1 |
| U | | | | | 6 | | | | 6 | | | | | 6 | | | 6 | 6 | | 6 | | | 1 | #6 | | | | 8 | #9 | | | | 6 | 6 | | | | | | | 6 | | | 1 | |

**Notes**. The following notations are used: 1, prediction for the compounds $ABPd_2$ with the Heusler-type ctystal structure; 5, prediction for a compound $ABPd_2$ with the $GdSnPt_2$ structure; 6, prediction for a compound $ABPd_2$ with the $YSiPd_2$ structure; 8, prediction for a compound $ABPd_2$ with the structure different from those given above; 9, prediction of the lack of a compound with the composition $ABPd_2$.

## V. Conclusion

Any field of scientific investigations passes a historical evolution sequence: from the collection and processing of the initial empirical data to the generalization of the experimental facts and the construction of scientific theories on their basis that reflect the fundamental relationships and links within the processes and phenomena under study. Such a sequence is also typical of the physical metallurgy: from the recipes of ancient metallurgists to the physical metallurgy of the 3rd millenium, which studies the structure and properties of metals and alloys, establishes the relationships with their chemical composition, structure and properties, as well as the regularities in their variation under the influence of external factors. Despite the progress in the modern physical metallurgy in the understanding of chemical and physical processes occurring in the metal systems, this science remains largely experimental. The methodological basis of the metal sciences is the physicochemical analysis of the metallic systems, *i.e.*, the systematic investigation of the physical properties of alloys depending on the variation of their chemical and phase composition.[2]

The progress in theoretical physics (the development of the band theory, the density functional theory, molecular dynamics *etc.*), the development of numerous softwares for the quantum chemical calculations and the availability of powerful computers are the factors determining the progress in the modern physical metallurgy. Scientists are attempting to apply the methods of quantum mechanics for the development of novel metals and alloys. It should be noted, however, that at present the theoretical physics can only explain the known facts, but it cannot predict the alloys not yet synthesized and intermetallic compounds with predetermined properties. Such situation is largely explained by the complexity of the condensed metallic systems.

Taking into account the above facts, it is clear why materials scientists apply empirical and semiempirical regularities that allow, to some extent, predicting the structures and properties of metals and alloys, instead of the accurate mathematical models. A certain criterion of the classification inferred from the experimental data corresponds to these regularities. The examples for the classification regularities include the well-known Darken–Gurry and Hume-Rothery rules for the prediction of the mutual solubility of metals, the Matthias criterion for the prediction of new superconductors with the crystal structure of the A15 type, the Laves rule for the prediction of the crystal structure for some intermetallic compounds *etc*. The classification of the diagrams of state underlies even the physicochemical analysis method.

It should be noted that the substitution of the empirical classification schemes for the functional relationship models based on physical theories and precise mathematical apparatus is typical of the majority of natural sciences. The classification has two aspects:[144] on the one hand, this is a cognitive process, which includes the creation of a classification scheme, *i.e.*, the ordering of the experimental data, the division of the multitude of observations into classes, the formulation of the differences between them, the formation of the concepts, and, on the other hand, this is the recognition process, *i.e.*, the determination of the status of a new object or a phenomenon in the classification scheme already built.

The progress in the development of the empirical classification criteria was attained with the application of the pattern recognition methods.[11] The use of computer programmes for the search of the multidimensional classification regularities in big arrays of updated experimental information allowed sharp reduction of time and costs of the development of new, and reconstruction of old, criteria. In contrast to the simplest empirical criteria developed on the basis of the analysis of a limited number of properties of chemical elements or analytical functions of these properties, the criteria formed by the computer programme allow selecting any number of the component properties for their inclusion into the multidimensional classifying regularity. The forms of the representation of the classification rules found by the computer programme can be different; this can be the analytical functions, neural or growing pyramidal networks, logical expressions, *etc*. In many cases, the perception, complete physical interpretation and analysis of the classifying regularities obtained with the use of a computer are very difficult for humans.

The problem of analysis and prediction of the systems not yet investigated is usually solved by a computer, while a human obtains the final result after the input of the components designation of the chemical systems. It is natural that the classifying regularities found are not fundamental laws of nature. They just point to the existence of regions of existence of different classes of chemical systems in the multidimensional space of the component properties, and the prediction, in this case, is limited to the search for the analogues of the systems not yet synthesized among those already studied.

Is it possible to discover a new phenomenon with the help of the programmes for the search of the multidimensional classification criteria? Surely, not. The classification regularities are rigidly bound to the concepts and theoretical representations that are currently used in chemistry and materials science. This fact defines both the problem statement of the chemical system classification, the choice of properties of the components for their description, the interpretation of the obtained results and the ambiguity and inaccuracy of the predictions based on the already existing concepts and ideas. For example, such a key concept in chemistry as 'compound' is vague like many other concepts formulated by a human being. It is not always possible to draw a distinct line between, for example, ordered solid solutions and disordered compounds based on the classification of compounds into daltonides and berthollides used in the physicochemical analysis. Moreover, the condition of the thermodynamic equilibrium for the construction of the diagrams of state is very rarely fulfilled in the investigation of the metallic systems, which produces unreliable results.

The classification rules obtained by both a human being and a computer are always incomplete since the principal concepts in chemistry are not very precise (vague) and experimental errors are present in the training sets. Therefore, the predictions based on these rules cannot be absolutely reliable. However, it is much easier and faster to re-establish the classification criteria with the help of a computer by including, into the computer learning, information on the chemical systems that contradict the available classification rules.

Thus, when predicting intermetallic compounds with the help of programmes of computer learning for pattern recognition, one succeeds in finding sophisticated multi-

dimensional classifying regularities in huge experimental data file for the metallic systems already studied. These regularities are used in undertaking predictions of systems with and without formation of compounds, in gaining predictions for the intermetallic compounds with predetermined compositions and with a certain crystal structure type under specified conditions, as well as in estimating their physical properties (melting point, superconducting transition temperature, *etc*.). In the prediction, it is only information on the properties of the components of the systems not yet studied that is used. As a result, the formation of hundreds of new intermetallic compounds was predicted. A comparison of the predictions with the experimental data has shown that the average accuracy of the prediction of the metallic and other inorganic compounds exceeds 80%.[11] The key conditions for the successful application of the methods of computer design of intermetallic compounds are the necessity of the existence of compact regions in the space of the properties of the components that correspond to different classes of metallic systems and the availability of the sufficient quantity of the experimental data for computer learning.

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