

# Prediction of the Types of Crystal Structure for $ABX_2$ ( $X = \text{Fe, Co, Ni}$ ) Intermetallics

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**Abstract**—A software package is developed to predict the types of crystal structures for ternary  $ABX_2$  ( $A, B$  are metals;  $X = \text{Fe, Co, Ni}$ ) intermetallics under normal conditions. These compounds are shown to be characterized by a Heusler-phase-type cubic structure. New  $ABFe_2$  Heusler phases are predicted for the first time.

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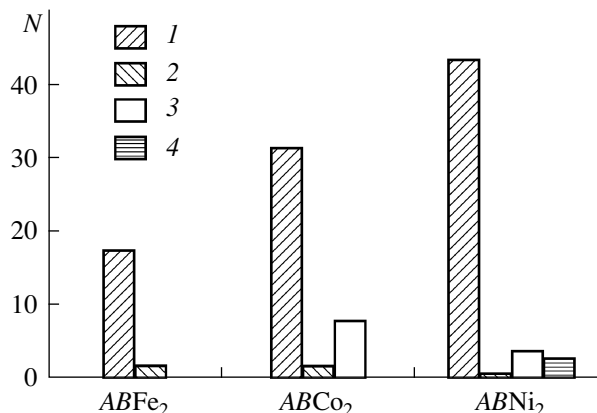
## INTRODUCTION

Being promising magnetic materials,  $ABX_2$  ( $A, B$  are metals or semimetals;  $X = \text{Fe, Co, Ni}$ ) compounds with an  $\text{AlMnCu}_2$  structure (Heusler phases) have long attracted the attention of researchers [1–8]. Keen interest in such phases in recent years is related to the creation of high-capacity magnetic storage devices, including spintronic devices [9–12].

## THEORETICAL ANALYSIS

More than 120  $ABX_2$  compounds have been obtained in  $A-B-X$  systems to date. Under normal conditions, most of them (about 100) have the a cubic  $\text{AlMnCu}_2$  structure (space group  $\text{Fm}\bar{3}\text{m}$ ; see figure). Crystal structures of the types  $\text{YSiRh}_2$  (space group  $P6_3/\text{mmc}$ ),  $\text{GdSnPt}_2$  (space group  $P6_3/\text{mmc}$ ), and  $\text{PrGaCo}_2$  (space group  $P\text{mma}$ ) form much more rarely. The authors of [13] believe that the criteria of Heusler phase formation are the atomic sizes of alloy components and the concentration of valence electrons per atom. When studying Heusler phases with lanthanides, the authors of [14] noted that the ratios of the atomic radii of components substantially determine the possibility of realization of  $\text{AlMnCu}_2$  structure type for  $\text{LnBX}_2$  compounds. However, Kiseleva [15] showed that the criteria proposed in [13] are insufficient to predict new Heusler phases, since the fields of stability of crystalline phases of different types are significantly intersected in diagrams whose coordinates are represented by an atomic radius and the concentration of valence electrons per atom. The fields of stability of crystalline phases of different types significantly are also intersected in the diagrams  $R_A/R_B - R_A/R_X$  and  $R_A/R_B - R_B/R_X$  ( $R_A, R_B,$  and  $R_X$  are the metallic radii

of elements  $A, B,$  and  $X$  forming  $ABX_2$  intermetallics) proposed in [14]. Therefore, Kiseleva [15] searched for criteria that included a wide set of the properties of components  $A$  and  $B$  (the ionization potential, the metallic radius, the entropies of individual substances, the melting point, the electron distribution over the energy levels of isolated atoms, and so on). She formed a multidimensional criterion to separate  $ABX_2$  ( $X = \text{Co, Ni, Cu, Pd}$ ) compounds with a Heusler-phase structure from compounds with other crystal structures and from systems having no  $ABX_2$  compounds under normal conditions. She used a special pattern recognition computer program intended for searching for complex regularities large volumes of experimental information [16]. In more than two decades, 20 predictions of cobalt- and nickel-containing intermetallics have been checked and have found that the



Bar chart for  $ABX_2$  compounds with crystal structures of the types (1)  $\text{AlMnCu}_2$ , (2)  $\text{YSiRh}_2$ , (3)  $\text{GdSnPt}_2$ , and (4)  $\text{PrGaCo}_2$ .  $N$  is the number of compounds.

**Table 1.** Predictions of types of crystal structure for  $ABFe_2$  compounds

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

Note: Designations: 1, Blank spaces compounds with a Heusler-phase-type structure; 2, compounds with a  $YSiRh_2$ -type structure; 4, compounds with a  $PrGaCo_2$ -type structure; and 6, nonformation of  $ABX_2$  compounds. Symbol # indicates systems information about which was used to teach a computer. Empty cells correspond to the noncoincidence of predictions obtained at different stages of prediction.

**Table 2.** Predictions of types of crystal structure for  $AB\text{Co}_2$  compounds

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

calculated results do not coincide with experimental data in six cases. We took into account the high average error of the computer prediction of Heusler phases (30%) and the fact that several tens of new compounds with such structures have recently been synthesized and decided to teach a computer using new data, a wider set of the properties of elements, and a more powerful set of pattern recognition programs. The purpose of this work is to revise the criteria of formation of  $ABX_2$  intermetallics with different types of crystal structure and to predict new Heusler phases in ternary systems with iron, cobalt, and nickel.

## EXPERIMENTAL COMPUTER TECHNIQUE

For computer analysis (computer learning), we used a specially designed information-analytical system, which included databases on the properties of inorganic substances and materials and a set of pattern recognition programs [17]. We analyzed information on 278 well-known  $ABX_2$  Heusler phases, 70 compounds with an  $\text{MgCuAl}_2$  structure, 38 compounds with a  $\text{GdSnPt}_2$  structure, 37 compounds with a  $\text{YSiPd}_2$  structure, 20 compounds with a  $\text{NaTl}$  structure, 11 compounds with a  $\text{PrGaCo}_2$  structure, 10 compounds with a  $\text{YSiRh}_2$

Table 2. (Contd.)

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

Note: Designations: 1, 2, 4, and 6, the same as in Table 1; 5, compounds with structures other than those given in Table 1.

structure, 16 compounds with structures other than these structures, and 486 cases of the absence of  $ABX_2$  compounds ( $A$  and  $B$  are various elements;  $X = Mg, Al, Fe, Co, Ni, Cu, Ru, Rh, Pd, Ag, Ir, Pt, or Au$ ). This information was extracted from database Phases on the properties of inorganic compounds (<http://phases.imet-db.ru>) [18].

Information on metallic systems was presented in a computer memory in the form of a set of the properties of chemical elements  $A, B,$  and  $X$  that included the following parameters: the pseudopotential radius (accord-

ing to Zanger); the enthalpy of vaporization; the melting, boiling, and Debye temperatures; the first three ionization potentials; the distances from valence and core electrons (according to Schubert); the ordinal number (according to Mendeleev–Pettifor); the electronegativity (according to Pauling); the Miedema chemical potential; the quantum number; the thermal conductivity; the group number in the periodic system; the molar heat capacity; the enthalpy of melting, vaporization, and atomization; the entropy of a solid state

**Table 3.** Predictions of types of crystal structure for  $ABNi_2$  compounds

Element <i>B</i>	Element <i>A</i>																	
	Li	Be	Mg	Al	Si	Sc	Ti	V	Cr	Mn	Fe	Co	Cu	Zn	Ga	Ge	Y	Zr
Mg	1																	
Sc			1	#1														
Ti	1			#1		1												
V	1			#1		1												
Cr				#1	6		6											
Fe		6	6		6		6	6	#6	#6								
Co		6	6		6		6	6	6	6	#6							
Cu		6	#6	#6	#6	5	5	6	6	#6	6	6						
Zn		6	#6							6	6	6	6					
Ga					1	#1	#1	#1		#1			6					
Ge	#1						1	1		#1				#1				
Zr	1			#1								#6	6		#1			
Nb	1			#1				6	6		6	6	#6		#1		6	
Ru		6	6	#6	6		#6	6	6	6	6	6	6	6		6	6	
Pd		6	6	6	6		6	6	6	#6	#6	#6	#6	6		6		
Ag		6			#6				6	6	6	6	#6	6	6			
In			#1			#1	#1	1	1	#1			6	6		1		#1
Sn	1	1	#1		6	#1	#1	#1	1	#1	6	6			#6			#1
Sb			#1				#1			#1	6		#1	6				#3
La			#1											2				
Ce				4										#2		2		
Pr																2		
Nd																2		
Pm															4	2		
Sm																2		
Eu																2		
Gd																2		
Tb																2		
Dy																2		
Ho																2		
Er																2		
Tm																2		
Yb																		
Lu																		
Hf				#1			#6								#1			
Ta		6	6	#1							6	6	#6		#1			
Pt		6	6		6		6	6	6	6	6	6	#6	6				6
Tl							1	1			6	6	6					1
Pb											6	6	6					1
Bi								1			6	6	6					1
Th											6	6	6					

phase; the atomic weight; the density; the linear thermal expansion coefficient; the metallic radius (according to Weber); etc. (in total, 108 parameters for each system). The data on the properties of elements were extracted from our database Elements (<http://phases.imet-db.ru/elements>). The initial information (learning set) for computer analysis consisted of a matrix each line of which corresponded to a set of values of the properties of elements forming a known chemical system and indicated to what class of systems it belonged.

To teach a computer, we used the following pattern recognition programs [19, 20]: an estimates calculation algorithm, a linear machine, a linear Fisher discrimi-

nant, logical regularities, a multilevel perceptron (inverse error distribution method), a  $Q$  nearest neighbor method, the support vector machine (SVM), statistically weighted syndromes, the method of binary decisive trees, the method of two-dimensional linear separators, and the method of inductive concept formation ConFor (which is based on growing pyramidal networks).

The prediction of the type of crystal structure of intermetallics included the following three stages:

(i) the prediction of  $A-B-X$  ( $A$  and  $B$  are various elements;  $X = \text{Mg, Al, Fe, Co, Ni, Cu, Ru, Rh, Pd, Ag, Ir,}$

Table 3. (Contd.)

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

Note: Designations: 1, 2, 4, and 6, the same as in Table 1; 3, compounds with a GdSnPt<sub>2</sub> type of structure; and 5, compounds with structures other than those given above and in Table 1.

Pt, or Au) chemical systems with the formation and nonformation of ABX<sub>2</sub> compounds;

(ii) multiclass prediction of the type of crystal structure (nine classes), namely, Heusler phases; compounds with NaTi, YSiRh<sub>2</sub>, MgCuAl<sub>2</sub>, GdSnPt<sub>2</sub>, YSiPd<sub>2</sub>, and PrGaCo<sub>2</sub> structures; compounds with structures other than these structures; and the cases nonformation of ABX<sub>2</sub> compounds;

(iii) sequential division of the systems into three classes, for example class 1 consisting of Heusler phases, class 2 consisting of compounds with structures other

than Heusler phases, and class 3 consisting of the cases where ABX<sub>2</sub> compounds are absent in an A–B–X system.

In all prediction stages, each pattern recognition computer program constructed a classifying regularity whose variables were represented by the properties of chemical elements, i.e., the components of A–B–X chemical systems. We used a cross-validation procedure to choose the most accurate programs for the prediction of new compounds [19]. In this procedure, given part of objects *f* (i.e., the descriptions of A–B–X systems as a set of the values of the properties of components) is removed from a learning set, a computer is taught on the remaining

objects, and the removed objects are used for examination recognition. The number of errors is fixed. The “control” objects are then returned to the learning set, and other  $f$  objects are removed from it. The procedure is repeated until all objects of the learning set play the role of control objects. With this procedure, we can objectively estimate the accuracy of a computer teaching algorithm for a certain learning set, especially in the case of pattern recognition methods, in which an undesired “overfitting” effect is observed. In this effect, an algorithm is only adjusted to a learning set and then gives bad results for new objects. After learning with cross-validation, we calculate the average examination recognition error and then use it to choose the best algorithms for collective decision making.

The aim of using the collective decision strategy is to increase the prediction accuracy. The idea of this approach is as follows. First, various algorithms of teaching a computer are independently applied to predict new compounds. The results of operation of some algorithms are then processed to form a final collective decision on attributing compounds to a certain class [19]. This use of “collective intelligence” often allows one to compensate for prediction errors induced by some algorithms. As a result, the most accurate result is obtained in most cases.

In the simplest collective decision method based on voting predictions, the result that is most often predicted by various algorithms is chosen. However, the predictions voting cannot always improve the reliability of prediction for very complex problems, especially in the case of weak execution of the main pattern recognition hypothesis, namely, the hypothesis of object compactness in the attribute space [19]. The most complex collective decision methods, such as the dynamic Woods method, the Bayesian method, a logic correction of sets of recognition algorithms, clustering and selection, decision templates, etc. [19], are intended for solving very complex prediction problems. These methods were used in our studies.

To find the best collective decision making algorithm, we recognized 100 objects chosen using a table of random numbers (uniform distribution), which were excluded from a learning set during both learning and collective decision making. At the final stage, the objects used to estimate the recognition quality were added to a learning set, and the process of constructing collective decision was again initiated with the chosen best algorithm. For prediction, we used the most “accurate” learning and collective decision algorithms. An unknown chemical system was attributed to a certain class via the insertion of the values of the properties of the elements that enter into the composition of this unknown metallic system into the found regularities. The final result of prediction was formed upon comparing the predictions obtained in all three stages.

## RESULTS AND DISCUSSION

Tables 1–3 give some results for the prediction of the type of crystal structure of  $ABFe_2$ ,  $ABCo_2$ , and  $ABNi_2$  intermetallics under normal conditions.

An analysis of Tables 1–3 demonstrates that no new iron, cobalt, and nickel compounds with crystal structures of the  $GdSnPt_2$ ,  $NaTl$ ,  $MgCuAl_2$ , and  $YSiPd_2$  types are predicted.

Results on predicting the types of crystal structures of  $ABRu_2$ ,  $ABRh_2$ , and  $ABPd_2$  compounds are presented in review [21].

## CONCLUSIONS

(1) We predicted the types of crystal structures of  $ABX_2$  ( $X = Fe, Co, Ni$ ) compounds in ternary systems. The calculations allow reduction of time and costs for search for new Heusler phases promising for designing magnetic materials.

(2) Ternary systems with iron, cobalt, and nickel are shown not to contain compounds with crystal structures of the  $GdSnPt_2$ ,  $NaTl$ ,  $MgCuAl_2$ , and  $YSiPd_2$  types.

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