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Application of a statistical model for predicting thermodynamic parameters for Laves hydride phases

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ABSTRACT

The statistical forecast model developed to optimize the process of searching for materials that meet the conditions of specific tasks of metal hydride technologies has been tested for application to the Laves phase alloys. The chemical and phase compositions of initial alloys were tested with X-ray and EDX. Absorption/desorption isotherm were measured and the experimental values of thermodynamic parameters compared with results of model calculations.

1. Introduction

Progress in the development of new composite materials used for the manufacture of cylinders for the storage of gases at high pressures has led to the appearance on the commercial market of cylinders containing compressed gases at pressures up to 80 MPa. Compressed hydrogen is the main working fluid of a number of technological processes, such as certification and recharging of standard (compression up to 30 MPa) and the latest carbon fiber-reinforced aluminium cylinders (compression up to 80 MPa), for stationary use (backup power supply of fuel cell systems), recharging of hydrogen tanks of mobile equipment (compression up to 80 MPa), catalytic hydrogenation processes in the food, pharmaceutical, petrochemical industries and many others. Compressing hydrogen to such high pressures by traditional methods is associated with high energy costs. Typical industrial reciprocating compressors with an output pressure of up to 40 MPa are equipped with engines with a power of 45–70 kW [1]. In addition, there is a risk of hydrogen contamination by oil vapour from the operation of the moving parts of such compressors. Metal hydride hydrogen compressors have a number of advantages over traditional compression methods, including simplicity of design and operation, no moving parts and assemblies, reliability and safety in operation, and the ability to use waste heat instead of electricity. Cost estimates for comparable metal hydride and mechanical compressors show their approximate equality. All this makes the task of developing metal hydride materials for an economical and safe technology of ultrahigh pressure hydrogen compression extremely urgent.

For these practical problems of metal hydride technology, the most suitable materials are multicomponent intermetallic compositions with the structure of hexagonal and cubic Laves phases. They have been the subject of research since the middle of the 20th century. The theoretical foundations and features of formation, as well as the practical use of Laves phases and their hydride phases are described in detail in a recent review [2]. The advantage of using precisely multicomponent metal compositions in metal hydride technology lies in the possibility of a precise change in operational properties (pressure of interaction with hydrogen at a given temperature) by replacing one or more metal components of the hydrogen storage alloy. However, such a variety of alloying components leads to a significant increase in the number of experiments in the search for a composition with specified operational parameters.

The metal hydride method of hydrogen storage has been known for a long time, and since the very fact of the ability of intermetallic compounds to reversibly absorb and release hydrogen at small changes in pressure or temperature has attracted increased attention of researchers. Any system for storing hydrogen in metal hydride is essentially a device for its compression, since when the system is cooled it is charged, and when the system is heated, hydrogen is supplied. Accordingly, the charge pressure will always be lower than the discharge pressure. The theoretical foundations and practical results of work in the field of metal hydride compression of hydrogen are most fully presented in recent reviews [3–5]. Scientific

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developments in this area have led to the creation of several tens of metal hydride hydrogen compressors (MHHC) with a calculated upper limit of the generated outlet pressure of 70 MPa at a temperature of 423 K [6–10]. It should be noted that in the developed compressors, an outlet pressure of more than 15 MPa is achieved only when using heat carriers with a temperature of more than 393 K (oil heating, electrical heating). The use of heating agents with temperatures up to 373 K leads to a decrease in the developed outlet pressure to 10 MPa. It is obvious that the use of electric heating significantly increases the cost of operating the installations. In addition, in the temperature range above 423 K, the undesirable process of hydrogen embrittlement of metal parts of the compressor begins more intensively. Reducing the risk of equipment hydrogen embrittlement is possible only by using special steels, which inevitably increases the cost of the final product. The disadvantages of developing alloy compositions for MHHC with an outlet pressure above 45 MPa include the fact that experimental tests of the achievable hydrogen desorption pressure have an instrumental limit of 30 MPa, and the choice of suitable compositions with an equilibrium pressure above 45 MPa is limited by calculations using the vant Hoff equation for already studied alloys at significantly elevated temperatures. As a result, the selection process of conjugated pairs of alloys for a multistage compressor will inevitably increase the number of experiments. Therefore, the task of developing a universal method for optimizing the selection of metal hydride materials capable of creating ultrahigh hydrogen pressure even at temperatures up to 373 K becomes extremely important for a wide range of practical problems.

In the process of accumulating knowledge in the field of the chemistry of intermetallic hydrides, in addition to obtaining experimental data, attention was paid to the development of approaches to the calculation and evaluation of the thermodynamic parameters of interaction with hydrogen, primarily the enthalpy of reaction and the decomposition pressure of hydride phases. A detailed analysis of the main methods of such calculations for the Laves phases is given in the fundamental review [11]. The results of the authors' statistical analysis of literature data on the reactions of hydrogen desorption by hydrides of Laves phases are also presented there. Unfortunately, these approaches do not allow one to select, on the basis of one's own calculations, such alloy compositions that satisfy the given pressure-temperature conditions. In the present work, we attempted to fill this gap.

2. Description of statistical model

According to Vegard's rule, the unit cell parameters change linearly depending on the composition of the solid solution. In practice, both positive and negative deviations from linearity are possible. It is known that for intermetallic compounds and alloys there is a proportional relationship between the equilibrium pressures of dissociation of hydride phases at a given temperature and the unit cell volumes of the initial alloys. Since, according to the van't Hoff equation, equilibrium pressures are determined from the values of the enthalpy and entropy of the alloy-hydrogen reaction, it can be assumed that Vegard's rule is also valid for the dependences of the enthalpy and entropy of the reaction on the concentration of alloy components. In the case of binary alloys, a preliminary calculation of the values of the thermodynamic parameters of the reaction is possible if the values of each of the parameters at the concentration boundaries of the solid solution are known. However, the introduction of even one alloying metal into the composition of the alloy significantly complicates such calculations. In practice, for more flexible control of the hydrogen sorption properties of alloys, it is necessary to introduce from two to six alloying components into the composition. Previously, we showed [12] that, with satisfactory reliability, the dependences of the enthalpy and entropy of reactions with hydrogen on the composition of alloys of the AB_5- type can be described by a complete polynomial of the second degree.

$$F(x) = Y_o + \Sigma A_i X_i + \Sigma B_{ij} X_i X_j \ (j \geq i) \quad (1)$$

where F(x) is the enthalpy or entropy of the (de)hydriding reaction of a particular alloy, X_i are the atomic concentrations of component metals of this alloy, Y_o, A_i, B_{ij} are the coefficients of the polynomial. F (x) and X_i are taken from literature data. Thus, we can compose a system of equations with unknown coefficients Y_o, A_i, B_{ij} for each type of multicomponent alloys or IMCs having the same crystal structure. This system is valid for the alloys of one series of continuous solid solutions. The determination of the coefficients of the polynomial is carried out by solution of a composed system of quadratic equations with respect to these coefficients. After determining the coefficients Y_o, A_i, B_{ij}, it becomes possible to calculate the values of enthalpies and entropies, and, consequently, the values of the equilibrium pressure of hydrogen at a given temperature for previously unexplored compositions. Further, by computer enumeration, it is possible to calculate the most probable alloy compositions that satisfy the predetermined ranges of the equilibrium pressure and reaction temperature values. The use of this statistical forecast model can significantly reduce the number of experiments required to select alloy compositions that satisfy the required pressure and temperature values for specific practical tasks of metal hydride technology. In order to check the applicability, we compiled literature databases on the interaction with hydrogen for alloys of structural types of Laves phases (C14 and C15) containing the following components: Ti, Zr, V, Cr, Mn, Fe, Co, Ni, Al, Cu. Currently, these databases contain: C14 absorption - 30 records, C14 desorption - 432 records, C15 absorption - 11 records and C15 desorption - 75 records. Such a disproportion between the amount of data on absorption and desorption is due to the fact that from the very beginning of the study of metal hydrides, researchers were mainly interested in desorption isotherms, considering them to be more consistent with the equilibrium state. The proposed model has an interpolation character, i.e. does not allow calculating the thermodynamic parameters of reactions for alloys containing metal components with a concentration exceeding the maximum value of this metal in the created base. In connection with this circumstance, in this work, we limited ourselves to calculating the parameters only for the reactions of hydrogen desorption by alloys of the C14 and C15 types. The number of base entries for C15 and C14 absorption reactions appears too small to obtain reliable results.

3. Alloy selection and experimental details

The main problem of creating such databases and obtaining correct results is establishing an exact correspondence between the thermodynamic data of reactions with hydrogen and the composition of the alloys. However, the prehistory of the studied samples, primarily the chemical composition of the alloy obtained after melting, is not always disclosed in the literature. This circumstance served as the main criterion for choosing the objects of study in this work. The first three alloys were chosen as a result of an attempt to reproduce the data of [13], in which the $Zr(V_{0.1}Ni_{0.55}Mn_{0.3}Co_{0.05})_{2.2}$ superstoichiometric alloy was studied. In our case three variants of the alloy were obtained by adding different amounts of manganese to compensate for its loss during melting. The fourth alloy was chosen according to the results of [14] as containing a significant amount of cobalt in its composition. The fifth alloy described in [15] attracted our attention due to its significant excess of stoichiometry. The sixth alloy was selected based on model calculations as having a design desorption pressure close to 80 MPa at 353 K and a maximum calculated compression ratio of 298 K. An alloy with these characteristics could serve as the working material of the last stage of a

Table 1
X-ray and EDX data of starting alloys.

Sample No.	Charge composition	EDX phase composition	a, Å	b, Å	c, Å	V, Å^3
1	$Zr(V_{0.1}Ni_{0.55}Mn_{0.3}Co_{0.05})_{2.2}$	C15 $Zr(V_{0.05}Ni_{0.55}Mn_{0.35}Co_{0.05})_{1.88}$ (96%)	6.927(7)	-	-	332.4(6)
		$Zr_7(Ni_{0.93}Mn_{0.06}Co_{0.01})_{11.26}$ (4%)	Traces			
		ZrO_2	Traces			
2	$Zr(V_{0.1}Ni_{0.55}Mn_{0.3}Co_{0.05})_{2.2}$	C15 $Zr(V_{0.12}Ni_{0.55}Mn_{0.27}Co_{0.05})_{1.98}$	7.057(5)	-	-	351.38(1)
		$Zr_7(Ni_{0.92}V_{0.01}Mn_{0.05}Co_{0.02})_{9.1}$	Traces			
		ZrO_2	Traces			
3	$Zr(V_{0.1}Ni_{0.55}Mn_{0.3}Co_{0.05})_{2.2}$	C15 $Zr(V_{0.11}Ni_{0.55}Mn_{0.29}Co_{0.05})_{1.93}$ (99%)	6.94(1)	-	-	334.0(9)
		$Zr_7(Ni_{0.82}V_{0.03}Mn_{0.12}Co_{0.3})_{9.76}$ (1%)	12.36(4)	8.75(3)	9.86(4)	1066(7)
		ZrO_2	Traces			
4	$Zr(Co_{0.5}Cr_{0.5})_2$	C14 $Zr(Co_{0.45}Cr_{0.55})_{1.9}$	5.02(2)	-	8.24(2)	179.9(9)
		$Zr_3Co_{0.99}Cr_{0.09}$ + $ZrCo_{0.85}Cr_{0.08}$	Traces			
		ZrO_2	Traces			
5	$ZrMn_{1.11}Fe_{1.22}$	C14 $Zr(Mn_{0.48}Fe_{0.52})_{1.95}$ (97%)	5.02(3)	-	8.22(3)	180(2)
		ZrO_2 (3%)	4.45(2)	-	4.97(2)	98.3(7)
6	$TiCr_{1.4}Mn_{0.2}Fe_{0.4}$	C14 $Ti(Cr_{0.71}Mn_{0.1}Fe_{0.19})_{1.94}$	4.8704(1)	-	7.9870(1)	164.078(3)

Table 2
XRD data of obtained hydrides.

Sample No.	Phase composition	a, Å	c, Å	V, Å^3	$\Delta V/V_0$, %
1	$Zr(V_{0.05}Ni_{0.55}Mn_{0.35}Co_{0.05})_{1.88}$	7.636(1)	-	445.3(1)	34.0
	$Zr_7(Ni_{0.93}Mn_{0.06}Co_{0.01})_{11.26}$	Traces			
	ZrO_2 (3.4%)	Traces			
2	$Zr(V_{0.12}Ni_{0.55}Mn_{0.27}Co_{0.05})_{1.98}$	7.566(6)	-	433.1(1)	23.3
	$Zr_7(Ni_{0.92}V_{0.01}Mn_{0.05}Co_{0.02})_{9.1}$	Traces			
	ZrO_2	Traces			
3	$Zr(V_{0.11}Ni_{0.55}Mn_{0.29}Co_{0.05})_{1.93}$	7.601(1)	-	439.1(1)	31.4
	$Zr_7(Ni_{0.82}V_{0.03}Mn_{0.12}Co_{0.3})_{9.76}$	Traces			
	ZrO_2	Traces			
4	$Zr(Co_{0.45}Cr_{0.55})_{1.9}$	5.390(1)	8.800(1)	222.0(5)	23.4
	$Zr_3Co_{0.99}Cr_{0.09}$ + $ZrCo_{0.85}Cr_{0.08}$	Traces			
	ZrO_2	Traces			
5	$Zr(Mn_{0.48}Fe_{0.52})_{1.95}$	5.470(4)	8.930(5)	232.0(3)	29.0
	ZrO_2	Traces			
6	$Ti(Cr_{0.71}Mn_{0.1}Fe_{0.19})_{1.94}$	5.2137(1)	8.5398(2)	201.0(1)	22.5

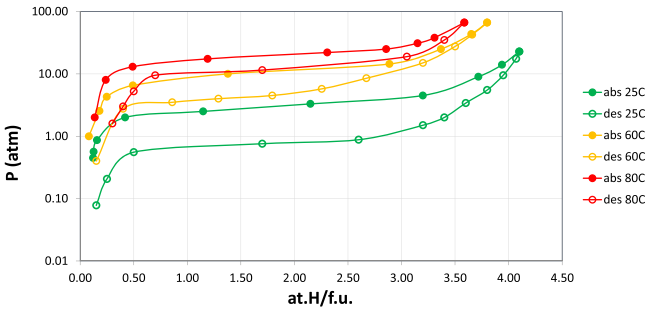

Fig. 1. Absorption/desorption isotherms for system #1-H_2.

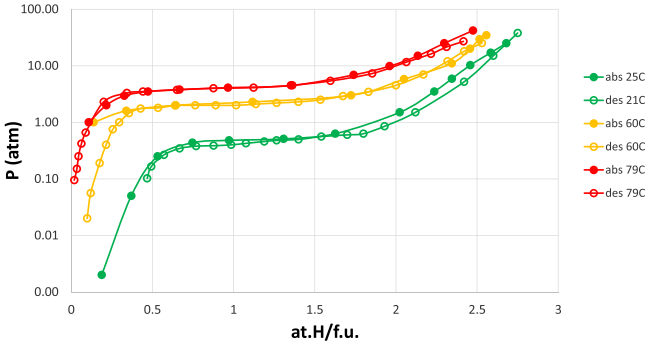

Fig. 2. Absorption/desorption isotherms for system #2-H_2.

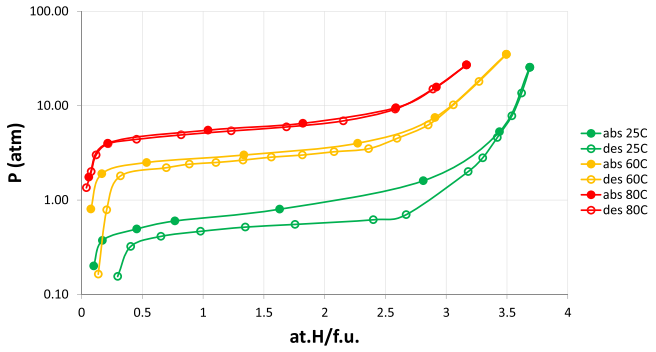

Fig. 3. Absorption/desorption isotherms for system #3-H_2.

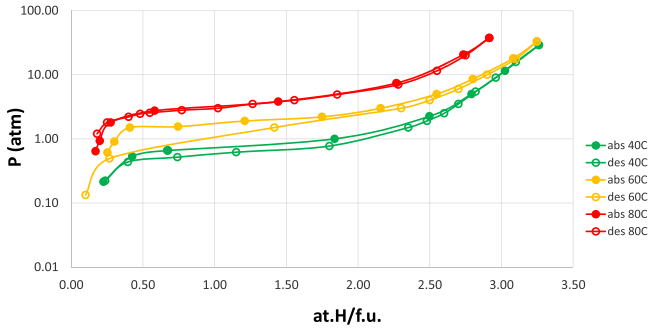

Fig. 4. Absorption/desorption isotherms for system #4-H_2.

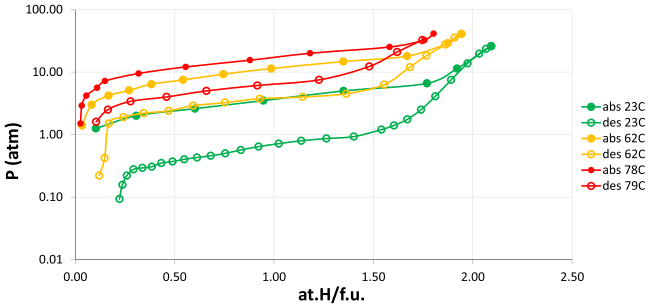

Fig. 5. Absorption/desorption isotherms for system #5-H_2.

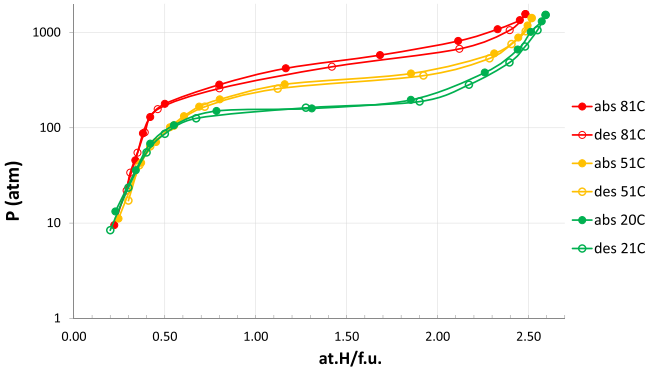

Fig. 6. Absorption/desorption isotherms for system #6-H_2.

metal hydride compressor for hydrogen charging of storage devices, designed for pressure 80 MPa.

Element metals used for preparation of alloys were of following purity: titanium – rod 99.6%, zirconium – rod 99%, manganese – rod 99.5%, vanadium – pieces 99.9%, chromium – rod 99.7%, nickel – wire reel 99.98%, cobalt – granular 99.99%, iron – rod 99.95%, copper – rod 99.99%. The alloys (about 15 g) were melted from component metals on a copper water-cooled electric arc furnace bottom in argon atmosphere 1.5 atm. The amount of manganese in the charge was taken with an experimentally determined excess to compensate for losses during melting. Annealing was carried out in a sealed evacuated quartz ampoule at 900 °C for 1200 h.

EDX was performed on a LEO EVO 50 XVP electron microscope. The method error is 5% of the determined value. X-ray quantitative phase composition and cell parameters of the obtained samples were carried out on an ARLX'TRA diffractometer using CuKα radiation. The accuracy of determining the cell parameters calculated using RIETAN2000 software is 0.01–0.05%.

Hydrogenation was carried out in a high pressure unit [16]. The samples were activated initially. This procedure included heating the sample up to 523 K in vacuum 10^{-2} Hg and hydrogenation by 10 MPa at room temperature repeated three times.

4. Results and discussion

Characteristics of the original alloys are presented in Table 1. The combined results of EDX and X-ray phase analysis (see Suppl.) show that all samples crystallize mainly in the cubic C15 or hexagonal C14 Laves phase. All samples are suitable for further study and possible addition to the databases, since they contain the main phase and small impurities that merge with background for X-ray patterns. Further, for calculations using the model, the compositions determined from the results of EDX for the main phases will be used (Table 1):

sample 1 - $Zr(V_{0.05}Ni_{0.55}Mn_{0.35}Co_{0.05})_{1.88}$;
sample 2 - $Zr(V_{0.12}Ni_{0.55}Mn_{0.27}Co_{0.05})_{1.98}$;
sample 3 - $Zr(V_{0.11}Ni_{0.55}Mn_{0.29}Co_{0.05})_{1.93}$;
sample 4 - $Zr(Co_{0.45}Cr_{0.55})_{1.9}$;
sample 5 - $Zr(Mn_{0.48}Fe_{0.52})_{1.95}$;
sample 6 $Ti(Cr_{0.71}Mn_{0.1}Fe_{0.19})_{1.94}$.

As far as possible, the X-ray analysis of the obtained hydrides was carried out to clarify their phase composition (Table 2). Before X-ray analysis of the hydride phase of the sixth alloy, as the least stable, it was stabilized with atmospheric oxygen at liquid nitrogen temperature.

To calculate the thermodynamic parameters of the reaction with hydrogen by the isotherms measurement method, the Van't Hoff equation was used: $RTlnP = \Delta H\text{-}T\Delta S$. Isotherms for all six alloys are shown in Figs. 1–6. Attention is drawn to the fact that all the investigated alloys exhibit insignificant hysteresis, which is practically absent in the case of alloys 2, 3, 4, and 6. This fact is important from the point of view of the practical application of alloys in various devices operating on the principle of metal hydride hydrogen storage. For samples 1 and 5, the hysteresis is larger at low temperatures. Since the phenomenon of hysteresis is usually associated with lattice relaxation, such a decrease in the hysteresis values can be associated with a greater mobility of atoms at high temperatures. As it was mentioned above, all the original samples were previously unexplored alloys and, therefore, it is rather difficult to compare their properties with tabular data. For C14 phases, results similar in trend for alloys 4–6 with relatively close compositions can be found in the tables presented in the review [11].

The results of the experimental calculation of thermodynamic parameters using the van't Hoff equation and the statistical model are presented in Table 3. Calculation and comparison of the equilibrium plateau pressures of hydrogen desorption was carried out for

Table 3
Experimental and calculated thermodynamic parameters of hydride phases.

Sample No.	Alloy composition	Desorption						Absorption	
		-ΔH (exp) kJ/ mole H_2	-ΔS (exp) J/ mole* K H_2	P, MPa			ρ	ΔH (exp) kJ/ mole H_2	ΔS (exp) J/ mole H_2* K
				T, K	Calc	Exp			
1	$Zr(V_{0.05}Ni_{0.55}Mn_{0.35}Co_{0.05})_{1.88}$ C15	**41.4 ± 0.3**	**137 ± 2**	**298**	**0.05**	**0.08**	**0.945**	**30.4 ± 0.2**	**113 ± 4**
				353	**0.67**	**1.07**			
2	$Zr(V_{0.12}Ni_{0.55}Mn_{0.27}Co_{0.05})_{1.98}$ C15	**33.2 ± 0.2**	**105 ± 2**	**298**	**0.04**	**0.04**		**35.5 ± 0.4**	**113 ± 2**
				352	**0.48**	**0.41**			
3	$Zr(V_{0.11}Ni_{0.55}Mn_{0.29}Co_{0.05})_{1.93}$ C15	**36.0 ± 0.1**	**116 ± 4**	**298**	**0.05**	**0.05**		**34.8 ± 0.2**	**113 ± 4**
				353	**0.49**	**0.56**			
4	$Zr(Co_{0.45}Cr_{0.55})_{1.9}$ C14	**38.8 ± 0.2**	**120 ± 2**	**313**	**0.1**	**0.07**	**0.998**	**35.1 ± 0.3**	**111 ± 3**
				353	**0.54**	**0.37**			
5	$Zr(Mn_{0.48}Fe_{0.52})_{1.95}$ C14	**35.5 ± 0.3**	**115 ± 3**	**296**	**0.08**	**0.05**		**24.6 ± 0.2**	**93 ± 4**
				352	**0.51**	**0.58**			
6	$Ti(Cr_{0.71}Mn_{0.1}Fe_{0.19})_{1.94}$ C14	**16.4 ± 0.1**	**98 ± 1**	**293**	**21.5**	**16.5**		**18.1 ± 0.1**	**105 ± 2**
				353	**77.8**	**44.5**			

two temperatures for each alloy. The pressure calculations according to the model were carried out separately for C14- and C15-type alloys. As follows from the data given in Table 3, the use of the proposed statistical model for estimating the thermodynamic parameters of reactions with hydrogen makes it possible to obtain quite acceptable results. This follows from the values of the Pearson correlation coefficients ρ for comparing the calculated and experimental pressures of hydrogen desorption by alloys of both types. Also, a comparison of the obtained Pearson coefficients, as expected, shows that the best correlation is given by calculations in the case when the database contains a larger number of records.

5. Conclusions

The applicability of the statistical model based on the Vegard rule and the van't Hoff equation for calculating the thermodynamic parameters of reactions with hydrogen was tested on the example of Laves hydride phases of structural types C15 and C14. The values of Pearson correlation coefficients (0.945 and 0.998) testify to the acceptability of the model for a preliminary assessment of the pressures of hydrogen desorption by C14- and C15-type hydride phases.

CRediT authorship contribution statement

S.Mitrokhin is responsible for the organization of research, model calculations, preparation of the manuscript. E.Movlaev is responsible for PCT measurements, M.Prokhorenkov is responsible for EDX and X-ray analysis.

Data Availability

No data was used for the research described in the article.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supporting information

Supplementary data associated with this article can be found in the online version at doi:10.1016/j.jallcom.2023.169802.

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