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Ti-based laves phase hydrides with high dissociation pressures

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Abstract

The interaction of Laves phase multicomponent alloys with hydrogen has been studied by means of P–C isotherms, X-ray, EDX and atomic adsorption analysis. The comparison of experimental and calculated parameters is discussed. The studied alloys can be employed in the thermosorption compressors.

Keywords: Hydrogen; Laves phases; Isotherms

1. Introduction

One of the problems arising in the design of metal–hydride devices is the availability of alloy hydrides having comparatively high hydrogen dissociation pressures and sufficient absorption capacities at ambient temperature. Multicomponent alloys based on Laves phases $TiCr_2$ and $TiMn_2$ can be rather useful from that point of view.

In the present work we have studied the interaction with hydrogen of several Ti-based Laves phases, which, according to calculations based on our model, described earlier [1,2], may be characterised by rather high hydrogen dissociation pressure at ambient temperature.

2. Results and discussion

Using our model we have calculated compositions for a series of alloys with potentially high hydrogen desorption pressure. The alloys have been prepared using a standard arc melting technique from metal components of purity higher than 99.9% The composition of alloys has been controlled by means of X-ray, EDX and atomic adsorption (AA) analysis. P–C-isotherms have been determined in a standard Sieverts type apparatus.

The compositions and characteristics of the starting alloys are presented in Table 1. According to X-ray and EDX analysis all the samples were mixtures of at least two phases. The main phase was always the C14 Laves phase. This is in good agreement with previous data [3]. The EDX-overall and AA compositions correspond to each other, while the composition of the matrix (main phase), as determined by EDX, is close to that of the alloying mixture of metal components (Table 1). The alloy compositions determined by different methods have been used for calculations of cell parameters and thermodynamical characteristics of desorption reactions.

The P–C isotherms are shown in Figs. 1–3. The experimental and calculated thermodynamical parameters of desorption reactions are presented in Table 2. Notable is the fact that Alloy 3 possesses the highest desorption

Table 1
Experimental and calculated characteristics of starting alloys

Composition	Tl	Zr	Mn	Cr	Fe	a (Å)	c (Å)	v (Å^3)
Alloy 1								
Experiment						4.877	7.98	164.4
Model	0.95	0.05	1.35	0.45	0.2	4.850	7.940	161.7
EDX	1.27	0.06	0.78	0.53	0.36	4.808	7.831	156.8
AA	1.08	0.06.	0.99	0.56	0.33	4.834	7.900	159.8
Alloy 2								
Experiment						4.876	7.999	164.7
Model	0.9	0.1	1.5	0.4	0.1	4.860	7.970	163.0
EDX	1.05	0.13	1.38	0.44	0	4.836	7.939	160.8
EDX–Matrix	0.93	0.14	1.4	0.53	0	4.853	7.973	62.6
AA	1.04	0.11	1.41	0.41	0.03	4.836	7.937	160.8
Alloy 3								
Experiment						4.854	7.949	162.2
Model	0.95	0.05	1.2	0.3	0.5	4.850	7.930	161.5
EDX	1.17	0.07	1.03	0.36	0.37	4.822	7.869	158.5
EDX–Matrix	0.79	0.08	1.1	0.45	0.58	4.875	7.975	164.1
AA	1.17	0.06	0.85	0.36	0.56	4.823	7.853	158.2

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Table 2
Experimental and calculated thermodynamical parameters of hydrogen desorption

	Alloy 1				Alloy 2					Alloy 3				
	Exp.	Model	EDX	AA	Exp.	Model	EDX	EDX–M	AA	Exp.	Model	EDX	EDX–M	AA
ΔH, kJ/mole H_2	19.2	22.3	17.2	19.5	18.3	24.9	25.7	26.6	25.2	16.4	17.4	17.8	17.8	15.1
ΔS, J/K·mole H_2	90.2	112.0	132.1	118.4	77.1	110.0	119.7	115.0	118.6	89.6	109.1	122.8	101.7	126.5
P_{293} atm	20.2	75	6807	514	5.8	20	58	19	51	57.2	404	1737	139	8287

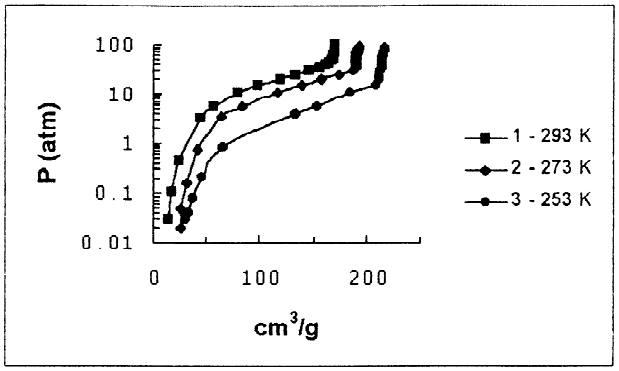

Fig. 1. Desorption isotherms for the system Alloy 1–H_2.

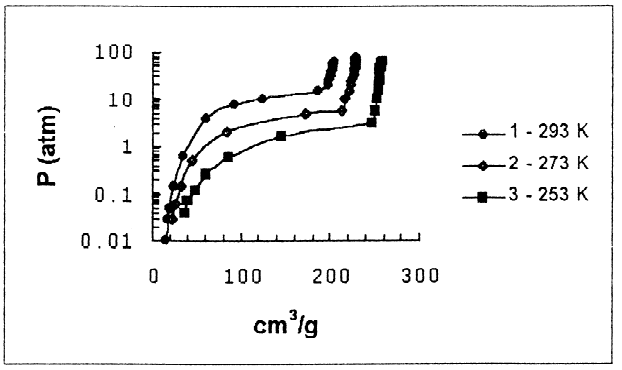

Fig. 2. Desorption isotherms for the system Alloy 2–H_2.

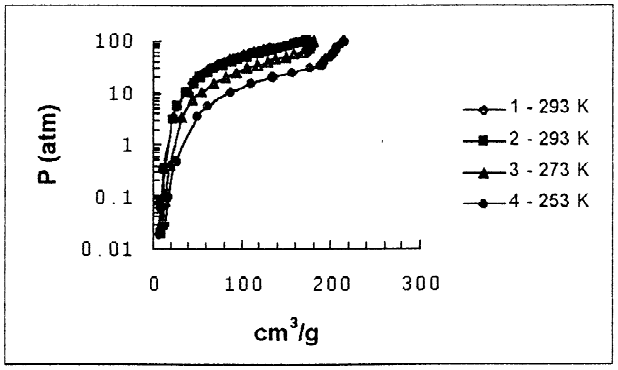

Fig. 3. Desorption isotherms for the system Alloy 3–H_2.

plateau pressure of all studied alloys. At ambient temperature and under a pressure of 100 atm, it is practically impossible to complete the absorption reaction. That suggests that the system Alloy 3–H_2 is characterised by a rather great hysteresis.

Analysis of experimental and calculated values of different characteristics suggests that the model gives an appropriate agreement of experimental and calculated parameters for alloys with correctly determined composition only within the concentration range of metal components taken as a computational base. Beyond this range there may be unpredictable deviations of calculated values from the experimental data.

The alloys studied in this and in previous [2] work may be of interest for the design of the thermosorption compressors.

Acknowledgments

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