ABOUT SPECIAL FEATURE OF THE SORPTION CHARACTERISTICS LAVES-PHASE BASED ALLOYS OBTAINED IN THE INTEGRATED SCALE

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The intensive development of researches in the area of hydrides of intermetallic compounds is caused both scientific interest and prospects of application of these compounds in metalic-hydrides technologies. It is possible already to choose composition of intermetallic compounds with the given properties (temperature and pressure of formation and decomposition of hydrides) for the decision of real tasks. Among intermetallic compounds with structure of Laves phases the practical importance has binary connection $TiMn_2$, its further perfection is possible by creation of multicomponent compositions with the help of alloying by d-transitive metals [1, 2]. Distinctive feature of these materials is the preservation of wide homogenous area at change of the contents of the basic components and of the alloying additives. Therefore was decided to smelt materials of some "average" composition incorporated the basic components Ti and Mn, and also alloying additives - Zr, V, Cr, Fe, Al.

There were used the alloys of the following composition: Ti - 28,0; Zr - 7,8; V - 5,5; Cr - 6,2; Mn - 45,5; Fe - 6,5; Al - 0,5 (wt.%). The alloys were melted in the induction vacuum furnace UPPF-2. The alloys were melted in alundum crucibles or crucibles from graphite MG-1. The order of charging of the initial components for all melting's was the following: iron, vanadium and zirconium together, chromium, manganese, titanium, aluminium. By x-ray-structures investigations was established, that the obtained alloys were single-phase and had a crystal lattice C14.

The chemical composition of alloys melted in alundum crucibles is closest to the initial composition. For obtaining a required composition of the alloy - store of hydrogen it is necessary to bring in corrective amendments to a initial composition. In view of physicochemical properties of elements it is possible to recommend to reduce the content of aluminium and to increase the content of zirconium. The characteristic of obtaining alloys and hydrides phases on their basis is given in tab. 1.

During melting process in the graphite crucibles occurs considerable magnification of carbon in the material (up to 2,1 % against 0,055 % for a malting in the ceramic crucibles). It was the reason that the material has ceased to be the alloy - store of hydrogen.

Table 1

The characteristics of alloys

Chemical composition of alloys (wt.%)		
Element	Crucibles material	
	Alundum	Graphite
Ti	27,63	29,51
Zr	5,99	5,77
V	5,65	5,78
Cr	6,3	5,55
Mn	45,01	44,63
Fe	8,08	7,57
Al	0,85	0,75
C	0,055	2,11
Crystalline structure		
Type of a lattice	C14	C14
a, Å	4,894	4,893
c, Å	8,017	8,019
c/a	0,6105	0,6102
Parameters of hydrogen sorption		
Equilibrium pressure H_2 (T=273 K)	12,0 atm	-
Equilibrium concentration H_2 (wt.%)	1,79	-
ΔH, kJ/mol H_2	28,0±2,0	-
ΔS, kJ/K·mol	120,0±6,0	-

A melting process in the large furnace was simulated. The material was melted in the composite crucibles. The crucibles consists from internal ceramic crucibles and external graphite one. The alloys melted in a such crucible, though had a little bit increased quantity of carbon (0,1-0,12 wt.%), had hydrogen capacity properties like to similar properties of alloys, melted in the ceramic crucible. So the equilibrium pressure of hydrogen at T=273 K was mattered P=10,0 atm, and quantity of the accumulated hydrogen H_2 at this temperature was at a level 1,70-1,74 (wt.%).

Is was established, that the material received by melting in the composite crucibles, is single-phase and has a crystal lattice C14. The repeated remelting of a material received in the composite crucible, does not give a significant changes of chemical and phase structures, hydrogen sorption properties. In tab. 2 the properties of hydrides phases on the basis of alloys obtained repeated remelting of a material after its synthesis in induction vacuum melting in a simple ceramic crucible (alloy 1) and in a composite crucible (alloy 2) are given.

Table 2.

The characteristics of alloys after repeated remelting

	Alloy 1	Alloy 2
Crystalline structure		
Type of a lattice	C14	C14
a, Å	4,83	4,85
c, Å	8,13	8,16
c/a	0,594	0,594
Parameters of hydrogen sorption		
Equilibrium pressure H_2 (T=273 K)	12,0 atm	15,0 atm
Equilibrium concentration H_2 (wt.%)	1,70-1,76	1,68-1,72
ΔH, kJ/mol H_2	32,0±2,0	25,0±2,0
ΔS, kJ/K·mol	134,0±6,0	113,0±6,0

References

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