CALORIMETRIC INVESTIGATION OF THE HYDROGEN INTERACTION WITH $Ti_{0.9}$ $Zr_{0.1}$ $Mn_{1.2}$ $V_{0.1}$

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Introduction

The investigation of the intermetallic compound (IMC)-H system, where IMC are the multicomponent compounds with overall formula (Ti,Zr)MnV nonstoichiometric composition with hexagonal structure C14 Laves phase forced us to think about the influence on the process of hydrogen interaction with IMC the deviation from stoichiometric composition AB_2.

The use of the twin-cell differential heat-conducting calorimeter Tian-Calve type permits to study of nature of hydrogen interaction with IMC more profound then it could be done by means of the method of P-C measurements, as we have a possibility to take the values of the partial molar enthalpies (ΔHdes.) of hydrogen interaction with IMC depending on hydrogen concentration in the IMC.

Results and disscusion

The intermetallic compound $Ti_{0.9}Zr_{0.1}Mn_{1.2}V_{0.1}$ with hexagonal structure C14 Laves phase was chosen for the research in present work. It is known [1] that in the substoichiometric compounds AB_2 type with Laves phase structure there is a rearrangement of A and B atoms among the crystallographic positions and the atoms of the A component partly occupy the positions of the B atoms, so the formula of the studied IMC can be rewritten as $Ti_{0.86}Zr_{0.14}Mn_{1.56}V_{0.13}Ti_{0.31}$. In this work all calculations were made exactly on this composition.

X-ray analysis showed that obtained sample of the IMC had hexagonal structure C14 Laves phase with lattice parameters: a = 4.932Å, c = 8.08Å and V= 170$Å^3$.

It should be marked that present IMC has very good hydrogen capacity (C=[H]/[AB_2]=3.25 at 25°).

In this present system at 76 - 95°C there are the large α-solid solution region of hydrogen in the IMC (≈ 0.5H at 76° C) and low equilibrium hydrogen pressure on plateau. Evidently it is connected with the large volume of the unit cell of the IMC (170$Å^3$) and with the fact that the positions of the B component partially are occupied by large amount of Ti and V atoms. It is known [2] that in the stoichiometric IMC with structure C14 Laves phase hydrogen atoms occupy tetrahedral interstitial sites [A2B2], however, in this case some of the B positions occupied by Ti and V atoms, which have a large affinity to hydrogen, so the part of the interstitial sites [A2B2] transformed into [A3B].

In contrast to $Ti_{0.9}Zr_{0.1}Mn_{1.5}V_{0.3}$ and $Ti_{0.9}Zr_{0.1}Mn_{1.5}V_{0.8}$ compounds, where we observed [3] the increase of ΔHdes. values with increasing hydrogen concentration in the IMC, that permitted us to suppose the existence two hydride phases in these compounds, in this case we assume that one hydride phase forms.

References

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