PHASE TRANSITIONS OF Ti_2Cu IN THE DESTRUCTIVE HYDROGENATION PROCESS

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Introduction

Destructive hydrogenation (DH) of the intermetallic compounds is a form of the extreme interaction with hydrogen because it is accompanied by the decomposition of the initial compound and by the formation of the new phases. At present this process practically is not investigated, although it is perspective for synthesis of the nanostructure composite materials. We suppose, that the known information about the synthesis of the direct hydride $Ti_2CuH_{2.7}$ is incorrect and needs the additional investigation.

Purpose of this work is to investigate the phase transitions during Ti_2Cu interaction with hydrogen.

Results and discussion

Thermodynamic estimations of possibility of Ti_2Cu direct and destructive hydrogenations have been carried out.

Table – Free Gibbs energies for reactions of Ti_2Cu direct and destructive hydrogenation

Reactions	-ΔG, kJ/mol at T, K		
	298	773	1273
$Ti_2Cu + 2.7H = Ti_2CuH_{2.7}$	490	335	170
$Ti_2Cu + 4H = 2TiH_2 + Cu$	983	784	576
$Ti_2Cu + 2H = TiH_2 + TiCu$	458	555	657

These reactions are shown to be thermodynamic allowed in temperature diapason from 298 K to Ti_2Cu melting point. The possibilities of the destructive hydrogenation reactions are predominate at the whole diapason of researched temperatures. Change of priority is thermodynamically impossible.

The objects of the experiment were the polished Ti_2Cu plates. Ti_2Cu was obtained from iodide titanium and reduced copper by the melting under argon atmosphere. Samples were hydrogenated at temperatures of 293–973 K under hydrogen pressure 1.0 MPa.

The powder patterns of Ti_2Cu DH products at 293, 373, 473, 573, 773 and 973 K under hydrogen pressure 1,0 MPa during 120 hours are presented on figure. As follows from the picture Ti_2Cu DH reaction at room temperature didn't pass. After Ti_2Cu DH at 373 K the phase with the tetragonal body-centered structure was detected, that, probably, corresponds to the hydrogen solution in β-titanium. When DH temperature increases up to 473 K, titanium hydrides and hydrogen solution in β-titanium were registered. Incompleteness of DH reactions at 373 and 473 K can be explained by the low rate of the reaction because of deceleration of the surface processes at these temperatures. DH reaction of Ti_2Cu at 573 and 773 K passed quite with the formation of titanium hydride and copper, and besides amount of copper increases with temperature enhance. Products of DH at 973 K were titanium hydride and β-$TiCu_3$ intermetalic compound. Final product, copper, was not registered, apparently, due to concurrent effect of the surface oxidative processes with the increase of temperature. Formation of oxides, which block hydrogen dissociation centers on the surface, reduces to slowdown of the destructive hydrogenation reaction.

The phase mechanism of Ti_2Cu destructive hydrogenation has studied by small step hydriding of the initial alloy at temperatures of 298 – 973 K. It is determined that the selective hydrogenation of titanium during Ti_2Cu DH is realized according to the scheme:

$$\beta\text{-}TiH_y\ (bcc) \rightarrow TiH_{1,924}\ (fcc) \rightarrow TiH_2\ (tetr.)$$

The copper-riched intermetallic phases are formed after leaving from the initial alloy as many. titanium as it is needed for the formation of new stochiometric titanium-copper ratios in accordance to Ti-Cu state diagram.

Conclusions

It is shown that Ti_2Cu interaction with hydrogen passes in the destructive hydrogenation field. The destructive hydrogenation is realized at temperatures of 293, 373, 573, 773 and 973 K and its products are titanium dihydride and copper.

Mechanism of Ti_2Cu DH is as follows: hydrogen selectively reacts with titanium which is left from composition of Ti_2Cu till to formation of titanium hydride. The copper-rich intermetalic phases form after leaving from the initial

alloy as many titanium as it is needed for the formation of new stochiometric titanium-copper ratios in accordance to Ti-Cu state diagram.

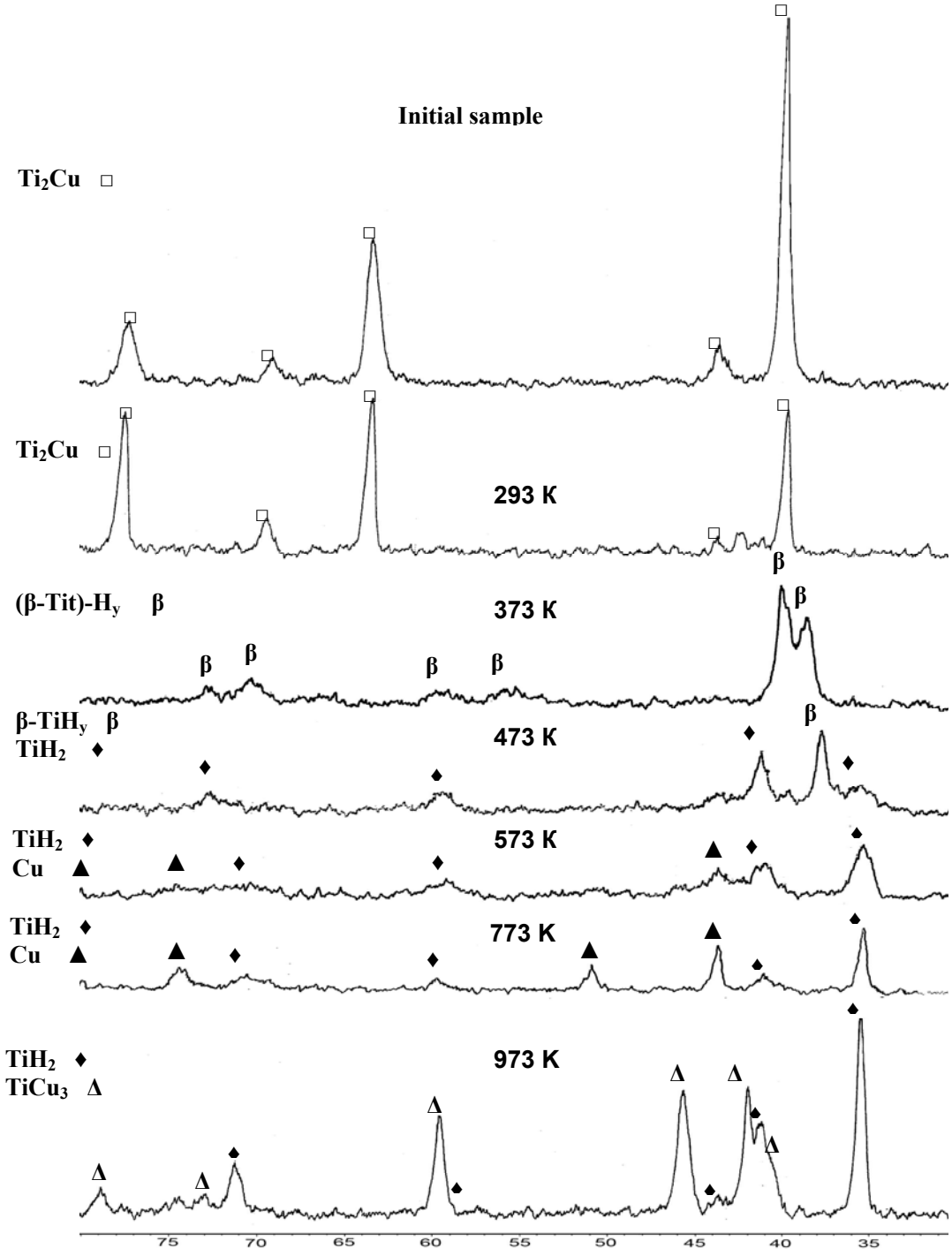

Fig. 1. The Products of Ti_2Cu phase transformation trough the destructive hydrogenation under hydrogen pressure of 1,0 MPa at temperatures of 293, 373, 473, 573, 773 and 973 K.