STRUCTURE OF RNi_3 (R-Ce, Ho)-BASED INTERMETALLIC HYDRIDES WITH DIFFERENT ANYSOTROPY OF THE LATTICE AT 5K AND 293K TEMPERATURE

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Intermetallic compounds (IMC) are materials for compact and safety storage of the hydrogen. These materials can be using for the development of hydrogen energy. The group of RNi_3 (R-Ce, Ho)-based compounds is also interesting for application as reversible hydrogen accumulator under soft pressure and temperature [1]. These compounds crystallized in $PuNi_3$ (space group *R-3m,* No *166*) and $CeNi_3$ (space group *$P6_3/mmc$,* No *194*) structure types. Both these structures are hybrid and consists of structural slabs with RT_2 ($MgZn_2$ structure type) and RT_5 ($CaCu_5$ structure type) composition, arranging in the direction perpendicular of the *z* crystallographic axis. Through the process of interaction of the hydrogen with intermetallic compounds and hydride phase formation, atoms of the hydrogen occupy interstitial sites in the crystal lattice. The crystallographic positions, occupied with hydrogen atoms, form several hydrogen sublattices in the structure of hydride [2]. The reaction of hydrogenation, when hydrogen atoms occupy sites in hydrogen sublattice, can lead to formation of the different hydride phases. In some cases, on cooling down of hydride sample, there may be decomposition this hydride into several new hydride phases. These transformations during lowering of temperature occur due to the redistribution of the hydrogen atoms in the sites of hydrogen sublattices. In early literature works, this redistribution of the interstitial atoms at low temperature was detect in the hydrides of *d*-metals [3]. In this work showed, that such behavior of hydrogen in the crystal lattice described with good agreement using of the lattice gas model. The RNi_3(R- Ce, Ho)-based hydride samples with medium hydrogen content (3.0-4.0 H/IMC) during lowering of the temperature also can decompose into several hydride phases. These new hydrides after heating back up to the room temperature transformed into phases with low stability. In literature is describe, that stability of hydrides might be different: the high stable hydrides not desorb of hydrogen at increased temperature, while the hydrides with low stability desorbs easy all hydrogen yet at the room temperature [4]. As was reveal RNi_3 (R- Ce, Ho)-based hydrides have different anisotropy of their crystal lattice [5]. More pronounced anisotropy was observe for hydrides containing R-metal of the cerium subgroup. Hydrides with R-metal of the yttrium subgroup have lattice with the small anisotropy. At the same time RNi_3(R- Ce, Ho)-based hydrides with low hydrogen amount (about of 1.0 H/IMC) have crystal lattice with small expansion and anisotropy. When these hydride samples were cooling down and heating back up to the room temperature, they rapidly desorbed all hydrogen. It was observe for both types of hydride samples, containing both cerium and holmium metals. The study of the RNi_3 (R- Ce, Ho)-based hydride structure with medium concentration was describe well in work [6]. In this work was reveal, that atoms of the hydrogen mostly occupy interstitial sites in the slabs with RNi_2 composition, containing more amount of the R-metal. We can suggest that in these hydrides with low hydrogen content, distribution of the hydrogen atoms in the lattice would be analogical. In this case, the different anisotropy of the hydride lattice first will be depend from the hydrogen amount in these hydrides. In structure of the RNi_3 (R- Ce, Ho)-based hydride with medium concentration, hydrogen atoms are ordered and have long-rang interaction each with other. In the structure of

hydride phases with low hydrogen amount, hydrogen atoms are as a disordered interstitial solution, without any interaction. At the same time, cooling down of the hydride samples with low concentration accompany with the hydrogen atoms redistribution in the hydrogen sublattices. This process may leads to possibility of appearing of the long-range interaction between atoms of hydrogen. For better understanding this behavior of hydrogen in the crystal lattice, it is necessary to perform the study of their structure. The most reliable method of the hydride structure study is neutron diffraction. At present work using neutron diffraction method were study samples of the RNi_3 (R- Ce, Ho)-based hydrides containing about of 1.0 H/IMC and having small lattice anisotropy at 5K and 293K temperature. For this study, samples with deuterium were prepared. Using of deuterium allows decreasing of the incoherent neutron scattering and obtain spectra that are more appropriate for refining. Obtained neutron data allows to determinate site positions of the hydrogen atoms and monitoring hydrogen redistribution in the sites of the structure.

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