

STRUCTURAL STUDIES OF PSEUDOBINARY COMPOUNDS $R(\text{Cu}_{1-x}\text{Ga}_x)_2$ ($R=\text{La, Ce, Y, Tb, Ho, Dy, Pr, Nd}$) AND THEIR HYDRIDES

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Introduction

Transformations of structure with CeCu_2 and AlB_2 types into Fe_2P type have been observed during hydrogenation of the $R(\text{Cu},\text{Ni})_2$ pseudobinary compounds [1]. Ternary gallides CeMgGa ($M - \text{Mn, Co, Cu}$) depending on the kind of transition metal are characterised by different crystal structure and hydrogenation properties. Intermetallic compounds CeMnGa , CeCoGa and CeCuGa crystallize in MgCu_2 , CeCoAl and CeCu_2 structure types, respectively. These phases absorb hydrogen at room temperature and their hydrogenation capacity depends on the type of crystal structure. Thus, the structure of the $\text{CeCoGaH}_{3.0}$ and $\text{CeCuGaH}_{0.8}$ hydrides turns in hexagonal AlB_2 type, and the $\text{CeMnGaH}_{1.6}$ hydride is characterized by MgCu_2 cubic structure of an initial matrix [2]. In this work we represent the results of studies of crystal structure of pseudo-binary $R(\text{Cu}_{1-x}\text{Ga}_x)_2$ hydrides for some REM.

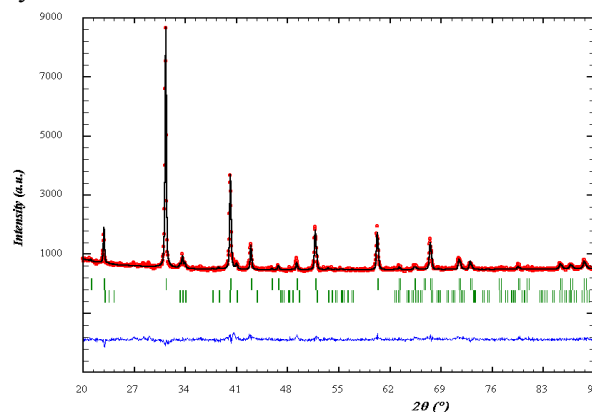
Results and their discussion

A number of gallides $R(\text{Cu}_{1-x}\text{Ga}_x)_2$ ($R = \text{La, Ce, Y, Tb, Ho, Dy, Pr, Nd}$) have been synthesized by arc melting method and annealed at 600°C during 700 h. The phase content and crystal structure of the parent alloys have been studied by X-ray diffractin analysis. It has been determined that the structure of the main phase belongs to CeCu_2 type. These phases absorbed hydrogen at room temperature and 0.1-0.12 MPa pressure of hydrogen after activation of samples in vacuum at 500°C during 15 minutes.

Intermetallic compound LaCu_2 has hexagonal structure of AlB_2 type, and other RCu_2 binary compounds as well as pseudo-binary compounds $R(\text{Cu}_{1-x}\text{Ga}_x)_2$ crystallize in orthorhombic KHg_2 (CeCu_2) type of structure. Our studies demonstrated that binary compounds LaCu_2 and TbCu_2 became amorphouse after the interaction with hydrogen. The crystal structure was not destroyed under influence of hydrogen for Ga-replaced samples.

Hydrogenation of $\text{LaCu}_{1.55}\text{Ga}_{0.45}$ and $\text{LaCu}_{1.4}\text{Ga}_{0.6}$ phases leads to the formation of the $\text{LaCu}_{1.55}\text{Ga}_{0.45}\text{H}_{2.55}$ and $\text{LaCu}_{1.4}\text{Ga}_{0.6}\text{H}_{2.45}$ hydrides with AlB_2 structure type. For these hydrides the refinement of crystal structure by Rietveld method

using FullProf software has been done. The experimental, calculated and differential profiles for $\text{LaCu}_{1.55}\text{Ga}_{0.45}\text{H}_{2.55}$ are presented in the figure, the positions of the peaks for main hydride phase and tracing amounts of parent compound are marked by vertical bars also.



Formation of the $\text{LaCu}_{1.55}\text{Ga}_{0.45}\text{H}_{2.55}$ and $\text{LaCu}_{1.4}\text{Ga}_{0.6}\text{H}_{2.45}$ hydrides is accompanied by increase in the unit cell volumes ($\Delta V/V$) on 17.2 and 14.6 %, respectively. Crystallographic parameters of the hydrides are presented in the table below.

Compounds	<i>a</i> , Å	<i>c</i> , Å	<i>V</i> , Å ³
$\text{LaCu}_{1.55}\text{Ga}_{0.45}\text{H}_{2.55}$	4.4884(5)	4.2071(4)	73.40(1)
$\text{LaCu}_{1.4}\text{Ga}_{0.6}\text{H}_{2.45}$	4.4549(2)	4.1751(3)	71.76(7)

Conclusions

Process of absorption of hydrogen by the $R(\text{Cu}_{1-x}\text{Ga}_x)_2$ ($R=\text{Y, REM}$) pseudobinary compounds under normal conditions occurs without amorphisation. The transformation of crystal structure from orthorhombic CeCu_2 into hexagonal AlB_2 type have been observed for $\text{La}(\text{Cu}_{1-x}\text{Ga}_x)_2$ phases with the small content of gallium during hydrogenation.

References

1. R.V.Denys, I.Yu.Zavaliy, R.Cerny, I.V.Koval'chuck. Structural studies of pseudobinary $\text{La}(\text{Cu}_{1-x}\text{Ni}_x)_2$ compounds and their hydrides. J. Alloys Comp., 2005, *in press*.
2. B.Chevalier, J.-L.Bobet, M.Pasturel, E.Gaudin, J. Etourneau.. Structure and magnetic properties of the ternary gallides CeMgGa ($M-\text{Mn, Co, and Cu}$) and their hydrides. J. Alloys Comp., 2003, 356-357: 147-150.