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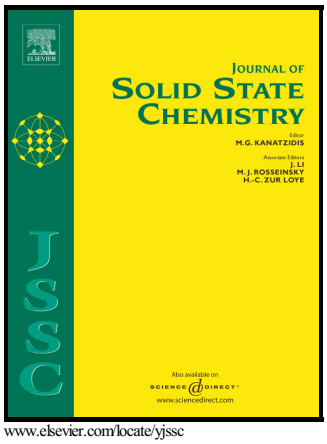

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PII: S0022-4596(15)30002-5
DOI: http://dx.doi.org/10.1016/j.jssc.2015.05.024
Reference: YJSSC18923

To appear in: *Journal of Solid State Chemistry*

Received date: 22 April 2015
Revised date: 19 May 2015
Accepted date: 23 May 2015

Cite this article as: V.V. Shtender, V. Paul-Boncour, A.B. Riabov, R.V. Denys and I.Yu. Zavaliy, Hydrogenation behaviour of the R_4MgCo (R=Y, La, ND, TB) compounds, *Journal of Solid State Chemistry,* http://dx.doi.org/10.1016/j.jssc.2015.05.024

Hydrogenation behaviour of the R_4MgCo (R = Y, La, Nd, Tb) compounds

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Abstract

The hydrogen absorption properties of the R_4MgCo compounds (R = Y, La, Nd, Tb; str. type Gd_4RhIn; sp.gr. $F\bar{4}3m$) have been studied for the first time. It was shown that their hydrogen storage capacity reaches about 2 wt. %. At low pressure hydrogenation and moderately elevated temperatures the formed hydrides preserve the original structure of the metallic matrix. The crystal structure of the R_4MgCoH_x hydrides have been determined by XRD. Experimental hydrogen storage capacity (12 at.H/f.u. for Y_4MgCo) is in good agreement with the theoretically calculated models, which allow also to estimate the distribution of H-atoms in metal lattice. TDS and DSC experiments demonstrated the multistep desorption process. XRD studies of the Tb_4MgCoH_x sample after TDS demonstrated the formation of TbH_2 as the main phase and disproportionation of the parent compound.

Keywords: Hydrogen storage, Metal hydride, Rare Earth compounds, Magnesium compounds, Crystal structure, Thermal desorption.

1. Introduction

Magnesium-containing alloys and intermetallic compounds are among the most studied hydrogen absorbing materials [1]. Magnesium is characterised by high capacity (7.6 wt. % H_2), but it has some drawbacks that limit its wide use as a medium for hydrogen storage and transportation. Intensive studies have been carried out on magnesium based composite materials, which have improved sorption-desorption characteristics [2–5]. It is shown that the addition of magnesium enhances hydrogen absorption properties of R–Ni alloys (R – rare earth metal) [6–11]. Magnesium-containing compounds $(R_{1-x}Mg_x)_nNi_m$ (n = 1, m = 2–3.5) are characterised by improved charge-discharge parameters and used as electrode materials for Ni/MH batteries [12, 13]. It has been shown also that the increase of cobalt content in the RMg(Ni,Co)$_4$ compounds results in the increase of hydrogen storage capacity [14–16]. These results caused the interest to other compounds in R–Mg–d-metal systems.

The R_4MgCo compounds (R = Y, La, Pr, Nd, Sm, Gd–Tm) were obtained for the first time by Tuncel et al. [17]. Their structure has been determined by single crystal method. It has been