STUDIES OF NOVEL HYDRIDES SYNTHESIZED UNDER HYDROGEN PRESSURE

Filipek S.M.,[1] Paul-BoncourV[2]., LiuR.S.,[3] SugiuraH.,[4] Tsutaoka T.,[5] MarchukI.,[1] Mylswamy S.,[3] Wierzbicki R.,[1] Sato R.[1]

[1] Institute of Physical Chemistry, Polish Acad. of Sci., Warsaw, Poland

[2]Laboratoire de Chimie Métallur. des Terres Rares, CNRS, 94320 Thiais, France

[3] Department of Chemistry, National Taiwan University, Taipei 106, Taiwan, ROC

[4]Graduate School of Integrated Sci., Yokohama City University, 22-2 Seto, Kanazawa-ku, Yokohama 236-0027, Japan

[5]Hiroshima University, Faculty of Education, Higashi-Hiroshima, Japan

[*]*Fax:+48-22-343 3334; E-mail: smf@ichf.edu.pl*

Several novel hydrides have been synthesized recently in the series of RT_2 Laves and R_7T_3 intermetallic compounds (where R - rare earth and T - transition metal). RT_2 Laves compounds crystallize in the cubic (C15, space group *Fd3m*) or hexagonal (C14, space group $P6_3/mmc$) structure while R_7T_3 crystallize in the Th_7Fe_3-type hexagonal structure in which R occupies three non-equivalent sites.

Compounds of both series display interesting magnetic properties with temperature-related anomalous phenomena.

It is well known that generally RT_2 Laves compounds easily absorb large amount of hydrogen even at moderate pressures. It was proved in many cases that interstitial hydrogen strongly modifies structural, magnetic and other properties of these compounds. Application of high hydrogen pressure resulted in formation of new hydrides with higher hydrogen content [2].

We expected that hydrogen should also markedly influence properties of R_7T_3 compounds.

Samples of parent materials were prepared by arc melting followed with annealing in vacuum. Synthesis of hydrides were performed in high pressure apparatus described elsewhere. Usually the syntheses were carried out at temperatures ranging from $100^0 - 300^0$ C.

We succeeded to synthesize two isostructural hydrides YMn_2H_6 [2,3] and $ErMn_2H_6$ (space group Fm-3m and lattice constants a=6.709(1) Å and a= 6.679(1) Å respectively) from starting materials of different structure (C15 for YMn_2 and C14 for $ErMn_2$). Both hydrides, with 6 H p.f.u., have the highest hydrogen content found so far in these intermetallics and both have the same (Fm-3m) space group. This structure forms through very strong rearrangement of metallic lattices which results in a partially disordered K2PtCl6 structure. According to our knowledge such kind of hydrides are for the first time derived from Laves intermetallics.

The surprising result was a disordered substitution of Y and Mn atoms on the 8c site in YMn_2H_6 (and seemingly Er and Mn in $ErMn_2H_6$). Interesting is the fact that such unusual hydrides were derived from different parent structures (C14 hexagonal and C15 – cubic).

Hydrogen concentration in hydrides formed from R_7T_3 intermetallics which we investigated so far reached 30 H atoms p.f.u. without change of crystalline symmetry; only expansion of lattice was observed. However, hydrogen absorption markedly changed magnetic properties.

Conditions of hydrides formation as well as their structural and magnetic properties are described and discussed. Equation of state was determined for some hydrides by using diamond anvil cell (DAC); pressure induced phase transitions were also found for several hydrides.

This work is a part of our systematic investigations of RT_2 and R_7T_3 intermetallics under high hydrogen pressure.

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