THE ELECTRONIC AND ELECTROCHEMICAL PROPERTIES OF THE $LaNi_5$-BASED ALLOYS

A. Szajek[a], A. Jezierski[a], M. Nowak[b], and M. Jurczyk[b]

[a]Institute of Molecular Physics, Polish Academy of Sciences, Poznań Poland

[b]Inst. of Materials Sci. and Engineering, Poznań Univ. of Technology, Poznań Poland

9.7 cm

$LaNi_5$-type alloys exhibit desirable electrochemical properties and are among the most promising electrode materials for nickel-metal hydride (Ni-MH_x) batteries. They crystallize in the hexagonal $CaCu_5$ structure and at room temperature can absorb up to 6 H/f.u.. Partial replacement of Ni by Al, Co, and Mn leads to an enhancement of the discharge capacity. Nanocrystalline $LaNi_5$-type materials have been prepared by mechanical alloying followed by annealing. The electrochemical properties have been investigated for the following matrials $LaNi_5$, $LaNi_4Al$, $LaNi_3CoAl$ *and* $LaNi_{15/4}Mn_{3/4}Al_{1/4}Co_{1/4}$. Changes in electronic structure are analyzed based on full-potetial local-orbital minimum basis bandstructure code FPLO [1], effects of chemical disorder in occupancy of 2c and 3g sites are considered within coherent potential approximation [2]. Total energy calculations allow predicting of site preference by Al, Mn and Co atoms in the $CaCu_5$-type unit cell. The impurities reduce the densities of electronic states at the Fermi level comparing to pure $LaNi_5$ compound.

[1] FPLO-5.00-18 improved version of FPLO code by K. Kopernik and H. Eschrig, Phys. Rev. B 59 (1999) 1743; http:// www.fplo.de

[2] K. Koepernik, B. Velicky, R. Hayn and H. Eschrig, Phys. Rev. B 55 (1997) 5717.

This work was supported by the Grant No. 3 T10A 033 29

13.4 cm

Subject category :

3. Magnetic Structure and Dynamics

Presentation mode :
poster

Corresponding author :
A. Szajek

Address for correspondence :
Institute of Molecular Physics
Polish Academy of Sciences
ul. Smoluchowskiego 17, 60-179 Poznań, Poland

Email address :
szajek@ifmpan.poznan.pl