THE ELECTRONIC AND ELECTROCHEMICAL PROPERTIES OF THE $\text{LaNi}_5$-BASED ALLOYS

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$\text{LaNi}_5$-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 $\text{CaCu}_5$ 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 $\text{LaNi}_5$-type materials have been prepared by mechanical alloying followed by annealing. The electrochemical properties have been investigated for the following materials $\text{LaNi}_5$, $\text{LaNi}_4\text{Al}$, $\text{LaNi}_3\text{CoAl}$ and $\text{LaNi}_{15/4}\text{Mn}_{3/4}\text{Al}_{1/4}\text{Co}_{1/4}$. Changes in electronic structure are analyzed based on full-potential 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 $\text{CaCu}_5$-type unit cell. The impurities reduce the densities of electronic states at the Fermi level comparing to pure $\text{LaNi}_5$ compound.


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