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

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9.7 cm

The battery electrode materials $La(Ni - Mn - Co - Al)_5$ are substitutional derivatives of $LaNi_5$ in which La occupies site 1(a), and Ni, Mn, Al, and Co sites 2(c) and 3(g) of space group $P6/mmm$. Nanocrystalline $LaNi_5$-type materials have been prepared by mechanical alloying followed by annealing. The amorphous phase forms directly from the starting mixture of the elements, without other phase formation. The as-milled powders were heat treated at $1000K$ for 0.5h under high purity argon to form the hexagonal $CaCu_5$-type phase. The powders were examined by XRD analysis, with Co K_α radiation, at the various stages during milling prior to and after annealing. The electrochemical properties of these materials have been investigated and discharge capacity enhancement has been observed. The electronic structure has been studied by the tight binding version of the linear muffin-tin orbital method in the atomic sphere approximation ($TB\ LMTO\ ASA$). The startting $LaNi_5$ is not magnetic but Al, Co, and Mn change band structure and in doped materials magnetic order is observed. The values of magnetic moments located on Mn atoms reach at leat $3\mu_B/atom$.

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