

Crystal structure and hydrogen sorption properties of the intermetallic $R\text{Y}_2\text{Ni}_{9-x}\text{M}_x$ phases ($R = \text{La, Pr, Nd}$; $M = \text{Cu, Co, Fe, Mn}$; $x = 0, 1, 2$)

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Modern society faces a significant challenge in the production, transportation, and storage of energy, a challenge exacerbated by worsening climate conditions stemming from the exploitation of fossil fuels such as coal, oil, and natural gas. As a result, there is increasing interest in harnessing renewable energy sources, like hydrogen, and in creating affordable and environmentally sound batteries for energy storage. The key factors driving the development of such batteries are high discharge capacity, cyclic stability, and cost-effectiveness. In this context, hydride-forming intermetallic compounds as negative electrode materials for nickel-metal hydride (Ni-MH) batteries have attracted significant research attention in recent years. Within the various classes of intermetallics demonstrating suitable hydrogen storage capabilities, pseudo-binary compounds with the PuNi_3 structure type have been extensively studied [1-4]. Yttrium- and lanthanum-based compounds are of particular interest due to their demonstrated acceptable high discharge capacity and cyclic stability.

Samples were prepared using arc-melting and annealing methods from pure metals. SEM, EDX, and XRD analyses were employed for alloy characterization. The hydrogen absorption properties of the selected alloys were characterized using a Sieverts-type apparatus. The samples were activated by heating to 300 °C under dynamic vacuum, then cooled to room temperature and subsequently hydrogenated with high-purity hydrogen gas (99.999%). The electrode materials were prepared by mixing powdered alloys with carbonyl Ni powder in a 1:3 ratio. This mixture was pressed into a pellet under a pressure of 10 tons/cm², and then sandwiched between two Ni foams with a fixed conductor. Electrochemical measurements were performed in a three-electrode cell using a potentiostat PGStat8 at a current density of 50 mA/g under ambient conditions. A 6M KOH solution served as the electrolyte, with Ag/AgCl (KCl saturated) as the reference electrode and a Pt counter electrode.

X-ray diffraction analysis revealed that the alloys formed as single-phase materials with either a PuNi_3 or LaY_2Ni_9 structure ($R\text{-}3m$ space group). Selected alloys were crushed into small pieces and then hydrogenated. The alloys readily absorbed hydrogen at room temperature and at a maximum pressure of up to 12 bar. Saturated hydrides of $R_2\text{YNi}_{9-x}\text{M}_x\text{H}_{10-14}$ preserved the parent structure when $M = \text{Cu}$ or Mn , but transformed into unknown structures when $M = \text{Co}$ or Fe . Electrochemical measurements revealed a variety of properties for the negative electrodes based on the $R_2\text{YNi}_{9-x}\text{M}_x$ alloys. Discharge capacities ranged from 150 to 350 mAh/g, and cyclic stability varied between 50% and 95%, depending on the R and M metals.

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