ELECTROCHEMICAL HYDROGENATION OF $Y_{17.5}Ti_{7.5}Ni_{62.5}Mg_5Al_{7.5}$ AND $Y_{17.5}Ti_{7.5}Ni_{62.5}Mg_5Sn_{7.5}$ ALLOYS.

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The global demand for accessible electrical energy is continuously increasing; therefore, the search for novel materials for reversible hydrogen storage remains a prominent area of research. RNi_3-type compounds belonging to the $PuNi_3$ structural type are highly effective at intercalating hydrogen atoms into the crystal lattice due to the presence of tetrahedral and octahedral interstitial sites, as confirmed by numerous studies [1]. Previous investigations [2–4] have demonstrated that $PuNi_3$-type compounds substituted with elements such as Ca, Ti, Mn, Mg, Co, Al, and Sn form hydrides with higher hydrogen capacity and exhibit enhanced cycling stability. The present work is devoted to the synthesis, phase composition analysis, and electrochemical hydrogenation of multicomponent alloys based on the YNi_3 compound doped with Ti, Mg, Al, or Sn.

Two samples $Y_{17.5}Ti_{7.5}Ni_{62.5}Mg_5Al_{7.5}$ and $Y_{17.5}Ti_{7.5}Ni_{62.5}Mg_5Sn_{7.5}$ were synthesized for the study by electric arc melting of metals (>0.999 mass fraction of the main component) under an argon atmosphere. For homogenization, the alloys were annealed in a muffle furnace at 400°C for two weeks, having been previously sealed in quartz ampoules under vacuum. The samples were quenched in cold water without breaking the ampoules. X-ray diffraction analysis (DRON-2.0M powder diffractometer, Fe$K\alpha$-radiation, $20° \leq 2\theta \leq 120°$, PowderCell-2.4 software) confirmed the presence of a phase with 1:3 stoichiometry and an orthorhombic $PuNi_3$-type structure (space group R-3m) as the major phase in all synthesized samples. The unit cell parameters of the main phase for $Y_{17.5}Ti_{7.5}Ni_{62.5}Mg_5Al_{7.5}$ are a = 0.49956(16) nm, c = 2.4361(12) nm, V = 0.5265(4) nm^3, and for $Y_{17.5}Ti_{7.5}Ni_{62.5}Mg_5Sn_{7.5}$: a = 0.49550(14) nm, c = 2.3831(10) nm, V = 0.5067(3) nm^3. Energy-dispersive X-ray spectroscopy (EDX) of the alloy cross-sections (Tescan Vega3 LMU scanning electron microscope, Oxford Instruments EDX system) confirmed the qualitative and quantitative composition of the identified phases for both samples. Electrochemical hydrogenation of the $Y_{17.5}Ti_{7.5}Ni_{62.5}Mg_5Al_{7.5}$ alloy (Swagelok two-electrode cell, MTech G410-2 galvanostat, charging time t_{ch} = 4 h, charging current I_{ch} = 1,0 mA) demonstrated efficient hydrogen intercalation, showing high efficiency η = 95 % (at the 15th cycle) and a discharge time t_{disch} = 3.8 h. Electrochemical investigation of the $Y_{17.5}Ti_{7.5}Ni_{62.5}Mg_5Sn_{7.5}$ sample under the same conditions showed an efficiency η = 90 % (15th cycle) and a discharge time t_{disch} = 3.6 h.

After 50 charge-discharge cycles, partial amorphization of the electrode material was observed for both samples, as evidenced by changes in grain morphology and composition; however, the crystalline structure of the material remained fundamentally unchanged. As expected, the unit cell volumes of the main phase increased for both samples. Specifically, the volume expansion was 5.8 % for the $Y_{17.5}Ti_{7.5}Ni_{62.5}Mg_5Al_{7.5}$ sample and 2.5 % for the $Y_{17.5}Ti_{7.5}Ni_{62.5}Mg_5Sn_{7.5}$ sample. Comparing the experimental results of both samples, it can be concluded that the $Y_{17.5}Ti_{7.5}Ni_{62.5}Mg_5Al_{7.5}$ composition exhibits a superior capacity for reversible hydrogen absorption.

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