ELECTROCHEMICAL SYNTHESIS OF HYDRIDES $Tb_2Ni_{16}SiH_x$ AND $Tb_2Ni_{16}Li_{0.5}Si_{0.5}H_x$

Kordan V. M., Nytka V. V., Tarasiuk I. I., Zelinska O. Ya., Pavlyuk V. V.
Department of Inorganic Chemistry, Ivan Franko National University of Lviv,
6 Kyryla i Mefodiya St., 79005 Lviv, Ukraine
kordan50@gmail.com

Doping components have the influence on structural, physical and chemical characteristics of the electrode materials. The material on the basis of multicomponent alloys often demonstrates better electrochemical characteristics than individual compounds. In this study we present our results of the the electrochemical hydrogenation of Tb_2Ni_{17} phases doped by silicon and lithium.

The samples were synthesized by arc melting of pressed pallets containing a mixture of pure metals with further homogenization annealing. The synthesized alloys were tested as anode materials in a Swagelok-prototype of Ni-MH batteries. As a negative electrode we used the powders of alloys with nominal compositions $Tb_2Ni_{16}Si$ and $Tb_2Ni_{16}Li_{0.5}Si_{0.5}$ that according to X-ray phase analysis contained only expected phases with Th_2Ni_{17}-type structure (space group $P6_3/mmc$) (see Table). As a positive electrode we used a mixture of $Ni(OH)_2$ and graphite powders for better conductivity. A separator soaked in electrolyte (6 M KOH) was placed between the electrodes. Electrochemical reactions that occurred on the electrodes were the following: $MH_z + zOH^- \xleftrightarrow{\text{discharge / charge}} M + zH_2O + z\bar{e}$ (anode); $NiOOH + zH_2O + z\bar{e} \xleftrightarrow{\text{discharge / charge}} Ni(OH)_2 + zOH^-$ (cathode).

Both materials can absorb 2.3-2.4 H/ f.u. Doping by Li and Si has improved Coulomb efficiency of the electrochemical hydrogenation for more than 3 % and increased capacity stability of the anode material with $Tb_2Ni_{16}Li_{0.5}Si_{0.5}$ (Figure).

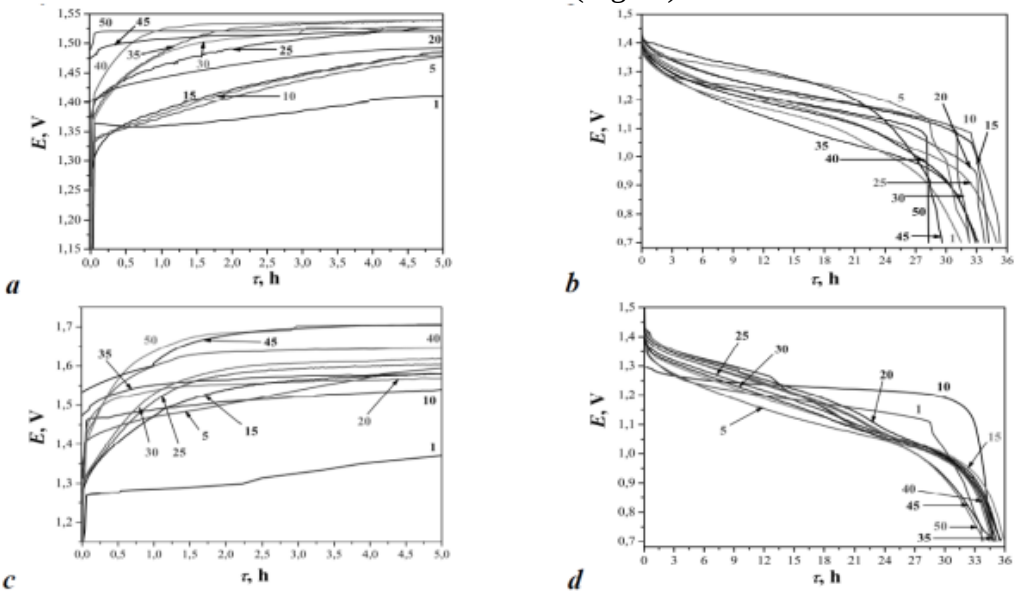

Fig. Selected charge and discharge curves for anode materials based on $Tb_2Ni_{16}Si$ (*a*, *b*) and $Tb_2Ni_{16}Li_{0.5}Si_{0.5}$ (*c*, *d*) phases

Table. The results of X-ray phase analysis and electrochemical hydrogenation of the $Tb_2Ni_{16}Si$ and $Tb_2Ni_{16}Li_{0.5}Si_{0.5}$ phases and their hydrides

Solid solution / hydride	*a*, Å	*c*, Å	*V*, Å^3	$\Delta V/V$, %	H_{charge} / f.u.	$H_{discharge}$ / f.u.	$\bar{Q}_{discharge}$, mA·h	η, %
$Tb_2Ni_{16}Si$	8.3055(4)	8.0377(6)	480.18(4)	1.81	2.40	2.27	12.80	85.3
$Tb_2Ni_{16}SiH_x$	8.3712(7)	8.055(1)	488.85(8)					
$Tb_2Ni_{16}Li_{0,5}Si_{0,5}$	8.3076(4)	8.0428(7)	480.73(5)	0.61	2.39	2.29	13.28	88.5
$Tb_2Ni_{16}Li_{0.5}Si_{0.5}H_x$	8.3209(7)	8.066(1)	483.65(9)					