SYNTHESIS AND X-RAY STUDY OF THE $Tb_2Ni_{17-x-y}Li_xMg_y$ SOLID SOLUTION

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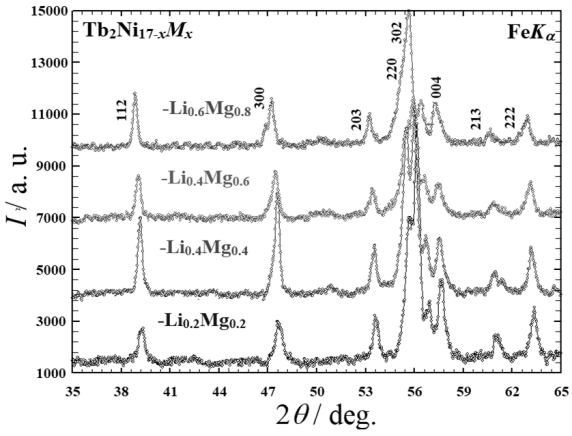
Systematic studies of the $Tb_2Ni_{17-x}M_x$ (M = *s*- and *p*-elements such as Li, Mg, Si, Sn, Sb) solid solutions showed that the maximal solubility of these doping components does not exceed 1.5–2 atoms per formula unit [1, 2]. The main reason for the formation of substitution solid solutions with small homogeneity range is different physical and chemistry characteristics, such as atomic radii and electronegativity of Ni, Li and Mg atoms.

The samples with nominal compositions $Tb_2Ni_{16.6}Li_{0.2}Mg_{0.2}$, $Tb_2Ni_{16.2}Li_{0.4}Mg_{0.4}$, $Tb_2Ni_{16}Li_{0.4}Mg_{0.6}$, $Tb_2Ni_{15.8}Li_{0.6}Mg_{0.6}$, $Tb_2Ni_{15.6}Li_{0.6}Mg_{0.8}$ and $Tb_2Ni_{15}LiMg$ were synthesized by arc melting of pressed pellets containing a mixture of pure metals (5 wt. % excess of Li and Mg) with further homogenization annealing in evacuated quartz tubes at 400 ºC. X-ray phase analysis (DRON-2.0M, FeK_α-radiation) confirmed that an expected phase with Th_2Ni_{17}-type structure (space group $P6_3/mmc$) was formed in the five first alloys (with trace amount of Ni). In the last alloy we observed a mixture of phases with 1:5 and 2:17 stoichiometry. Increasing of unit cell parameters depends on the content of doping elements (see Fig.). We predicted that Ni atoms are substituted only by a (Li,Mg) statistical mixture because of similar atomic radii and chemical properties of Li and Mg (r_{Li} = 1.52-1.53 Å, r_{Mg} = 1.60 Å). Changing of the unit cell parameters versus nominal alloy composition is presented in Table.



Nominal alloy composition	Lattice parameters (Å/ Å³)
Tb_2Ni_{17}[2]	a = 8.3129, c = 8.0184, V = 479.87
$Tb_2Ni_{16.6}$–$Li_{0.2}Mg_{0.2}$	a = 8.3103(9), c = 8.030(1), V = 480.28(10)
$Tb_2Ni_{16.2}$–$Li_{0.4}Mg_{0.4}$	a = 8.3103(9), c = 8.0311(8), V = 480.32(8)
Tb_2Ni_{16}–$Li_{0.4}Mg_{0.6}$[2]	a = 8.3115, c = 8.0286, V = 480.32
$Tb_2Ni_{15.8}$–$Li_{0.6}Mg_{0.6}$	a = 8.3165(9), c = 8.029(1), V = 480.93(9)
$Tb_2Ni_{15.6}$–$Li_{0.6}Mg_{0.8}$[2]	a = 8.3129, c = 8.0384, V = 481.08

Fig. Selected XRD powder patterns of the $Tb_2Ni_{17-x}M_x$, M = (Li, Mg) solid solution

Table. Dependence of the lattice parameters of the solid solution versus alloy composition

[1] V. Kordan, O. Zelinska, V. Pavlyuk, V. Nytka, R. Serkiz. Electrochemical hydrogenation of $Tb_2Ni_{17-x}M_x$ (M = Mg, Sn) phases. Chem. Met. Alloys, 2016, 9(3/4), 153–157.

[2] V. Kordan, V. Nytka, G. Kovalczyk, A. Balinska, O. Zelinska, R. Serkiz, V. Pavlyuk. Influence of doping elements on the electrochemical hydrogenation efficiency of Tb_2Ni_{17}-based phases. Chem. Met. Alloys, 2017, 10(1/2), 61–68.

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