Poster

Crystal structure and hydrogenation properties of the Mg_6CoSn ternary compound

N. Pavlyuk[1], G. Dmytriv[1], V. Pavlyuk[1,2], H. Ehrenberg[3]

[1]Department of Inorganic Chemistry, Ivan Franko National University of Lviv, Kyryla & Mefodia str. 6, 79005 Lviv, Ukraine,

[2]Jan Długosz University in Częstochowa, Institute of Chemistry, al. Armii Krajowej 13/15, 42200 Częstochowa, Poland

[3]Karlsruhe Institute of Technology (KIT), Institute for Applied Materials (IAM), Hermann-von-Helmholtz-Platz 1 D-76344 Eggenstein-Leopoldshafen Germany

grygoriy.dmytriv@lnu.edu.ua

The intermetallic compounds based on magnesium are widely investigated now due to their very good hydrogen storage and electrochemical properties [1]. During the systematic study of Mg–Co-Sn alloys the tetragonal phase Mg_6CoSn was detected. The Mg_6CoSn ternary compound was prepared in a tantalum crucible in a resistance furnace with a thermocouple controller. A single crystal of Mg_6CoSn was investigated using an Oxford Diffraction Xcalibur3 diffractometer with CCD detector. The crystal structure was successfully solved by direct methods and refined in space group $P4_2cm$ (№101). The refined lattice parameters are a = 9.8372(6) Å c = 6.8541(5) Å, V = 663.27(9) Å^3. The starting atomic parameters were taken from an automatic interpretation of direct methods followed by difference Fourier syntheses using SHELX-97 package programs [2]. Finally, all parameters are refined to R_1 = 0.044 and wR_2 = 0.054 using 742 independent reflections with $I > 2\sigma(I)$ and presented in Table 1. The ternary stannide Mg_6CoSn is isostructural to the Y-phase with $Mg_{74.5}Ni_{14.5}Sn_{11}$ composition [3].

The prepared Mg_6CoSn sample was hydrogenated by hydrogen gas at a pressure up to 12 bar and a temperature of 573 K. At these conditions, Mg_6CoSn absorbs up to 1.5 wt% hydrogen. Crystallographic analysis of the structure made it possible to determine the geometrically acceptable coordinates of the sites that can be occupied by hydrogen, namely, 8*e* (0.010, 0.170, 0.270), 4*d* (0.620, 0.620, 0,680) and 8*e* (0.470, 0.130, 0.445). These coordinates are the centres of the tetrahedral (in 8*e*) and octahedral (in 4*d*) voids. By comparing the observed specific hydrogen storage capacity with the theoretical capacity (based on a full occupation of all voids) an exploitation of 70% could be realized. Further studies will elucidate how this efficiency is affected by the specific hydrogen loading conditions (like pressure and temperature, but also in dependence on particle size).

Table 1. Fractional atomic coordinates and equivalent isotropic displacement parameters (Å^2) for Mg_6CoSn

Atoms	Sites	*x*	*y*	*z*	U_{eq}
Sn	4*d*	0.17142(12)	0.82858(12)	0.6775(2)	0.0141(5)
Co	4*d*	0.3091(2)	0.6909 2)	0.4083(5)	0.0034(7)
Mg1	2*b*	½	½	0.4486(17)	0.005(2)
Mg2	8*e*	0.2385(5)	0.4767(5)	0.1921(11)	0.0128(12)
Mg3	2*a*	0	0	0.929(3)	0.037(3)
Mg4	8*e*	0.0341(6)	0.6564(7)	0.3909(10)	0.0185(15)
Mg5	4*d*	0.2248(10)	0.7752(10)	0.0778(17)	0.039(3)

[1] Larpruenrudee, P., Bennett, N. S., Gu, Y., Fitch, R., & Islam, M. S. (2022). *Scientific Reports*, 12(1), 13436.

[2] Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen,Germany.

[3] Boudard, M., Bordet, P., Vincent, H., & Audebert, F. (2004). *Journal of Alloys and Compounds*, 372(1-2), 121-128.

Research funding by National Research Foundation of Ukraine (2022.01/0064), Simons Foundation (Award Number: 1290588).