華南理工大學
South China University of Technology

16th International Symposium on Metal-Hydrogen Systems

MH2018

October 28-November 2, 2018
Guangzhou, China

Program Book

Abstract ID: 312

MH2018 28 Oct - 2. Nov 2018 Guangzhou, China

High Pressure Hydrides Formed by Metallic and Semiconductor (Ti/Zr,Sc)NiSn Alloys

V.A. Yartys[1], V.E. Antonov[2,*], V. Berezovets[1], R.V. Denys[1], V.I. Kulakov[2] and S.V. Mitrohkin[3]

[1]Institute for Energy Technology, Kjeller, Norway;

[2]Institute of Solid State Physics, Russian Academy of Sciences, Chernogolovka, Russia;

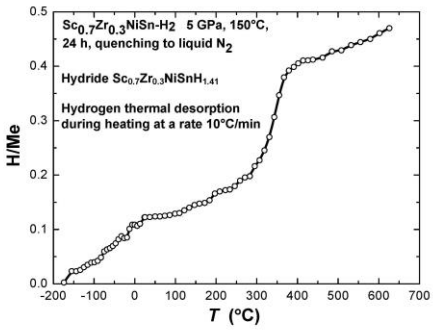
[3]Lomonosov Moscow State University, Moscow, Russia

antonov@issp.ac.ru; volodymyr.yartys@ife.no

Equiatomic TiNiSn and ZrNiSn intermetallics with a cubic FCC MgAgAs type of structure are semiconductors. In contrast, a chemically related ScNiSn of the orthorhombic TiNiSi type displays metallic conductivity. Because of the same metallic radii 1.60 Å of Zr and Sc and a similar atomic radius 1.47 Å of Ti, extensive solid solutions are formed between ScNiSn and ZrNiSn and between ScNiSn and TiNiSn. Increasing the content of Sc gradually decreases the resistivity of the alloys until a transition from the semicinductor to the metallic conductor occurs. Particularly, the homogeneous solid solutions $Sc_{0.7}Zr_{0.3}NiSn$ and $Sc_{0.6}Ti_{0.4}NiSn$ with the MgAgAs type structure are metallic. The objective of the current work was to examine the influence of the semiconductor-to-metal transition on the hydrogenation behaviors of the MgAgAs type alloys.

Two ternary intermetallics (ZrNiSn and TiNiSn) and two solid solutions ($Sc_{0.7}Zr_{0.3}NiSn$ and $Sc_{0.6}Ti_{0.4}NiSn$) were exposed to a hydrogen pressure of 5 GPa at 150 °C for 24 h and rapidly cooled to 100 K to prevent hydrogen losses in the course of further pressure release (the method is described elsewhere [1]). ScNiSn was saturated by hydrogen at a hydrogen pressure below 20 bar. The thermal stability and the total hydrogen content of the samples were determined by hot extraction performed from -186 to 650 °C [2]. In order to examine the process of thermal decomposition in more detail, in separate series of experiments, the heating was interrupted at different temperatures; the partly decomposed samples were quenched to the N_2 temperature and studied by X-ray diffraction at 85 K.

The figure shows typical hydrogen desorption trace for the hydrogenated $Sc_{0.7}Zr_{0.3}NiSn$ sample, which demonstrated a considerable H storage capacity of approx. 1.4 at. H/ f.u. and proved to be the most thermally stable. The $Sc_{0.6}Ti_{0.4}NiSn$ hydride had similar hydrogen capacity, but was less thermally stabile and mostly decomposed near 0 °C. The hydrogen content of the semiconductor intermetallics ZrNiSn or TiNiSn was much smaller and only reached ~0.2 at.H/f.u.



Reference:

[1] V.E. Antonov, B.M. Bulychev, V.K. Fedotov, et al. //Int. J. Hydrogen Energy 42 (2017) 22454.

[2] V.A. Yartys, V.E. Antonov, D. Chernyshov, et al.//Acta Mater. 98 (2015) 416.