Electronic structure and hydrogen absorption in Mg-Ni alloy thin films

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The strong interest in pure Mg and Mg-based alloys as hydrogen storage materials is associated with the fact that magnesium can absorb a large amount of hydrogen. Moreover, magnesium is abundant, light weight, and relatively not expensive [1]. Magnesium based thin film materials are subject of intensive studies due to a potential application as switchable mirrors and hydrogen sensors [1,2]. In this contribution we report on electronic structure and room temperature (RT) hydrogen absorption in Mg-Ni alloy thin films. Mg-based alloy thin films were prepared on transparent glass substrates at RT by UHV RF/DC magnetron co-sputtering. Before hydrogenation, all samples were coated with a 10 nm thick Pd layer. The chemical composition of all the layers and interface mixing between Mg-Ni and Pd layers were studied in-situ using X-ray photoelectron spectroscopy (XPS). Furthermore, the XPS valence bands were measured for all the prepared alloy thin films. Hydrogen absorption in Mg-Ni alloy thin films were studied at a pressure of about 1000 mbar using simultaneous optical transmittance and four-point resistivity measurements. Moreover, before and after hydrogen absorption the samples were characterised by Atomic Force Microscopy and high-angle X-ray diffraction (XRD). XPS measurements showed no surface segregation effect in freshly prepared Mg-Ni alloy thin films. On the other hand, successive measurements of the XPS Mg-2p, Ni-2p and Pd-3d peaks for Mg2Ni thin films covered by Pd layer revealed a formation of interface Mg-Pd alloy layer. Such an interface alloy layer can considerably influence on the hydrogen absorption in the Mg2Ni thin films [2]. Transmittance and resistivity measurements during hydrogen absorption showed that the 100 nm – Mg thin film covered by 10 nm Pd layer needed about 200 h for saturation. The MgNi and MgNi2 alloy thin films revealed no hydrogen absorption at RT. On the other hand, the fastest rise in transmittance was observed for Mg2Ni thin film covered by 10nm Pd. The transmittance of the sample with a thickness of about 200 nm reached 90 percent of the maximal value after 40 s of hydrogenation. The sample was completely loaded with hydrogen after about 20 minutes. RT hydrogen absorption in pure Mg and Mg2Ni alloy thin films was also confirmed by intense hydride reflections observed in the XRD patterns.

References:

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