Influence of valence band modifications on hydrogen absorption in Zr-Pd alloy thin films

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Intermetallic compounds based on hydrogen absorbing elements usually form stable hydrides. This is the case of $PdZr_2$ alloy. On the other hand, a similar compound, $ZrPd_2$, does not absorb hydrogen, although it has the same crystal structure and satisfy the empirical geometrical criteria for hydride formation. The above behaviour was explained as a purely electronic effect. In this contribution we study valence bands modifications of in-situ prepared nanocrystalline $PdZr_2$ and $ZrPd_2$ thin films using X-ray and ultraviolet photoelectron spectroscopy. Results were compared with valence bands calculated by ab initio methods. Furthermore, hydrogen absorption and desorption kinetics up to 1000 mbar were studied in Pd covered samples. Results showed that modifications of the valence bands of the nanocrystalline alloy thin films could significantly influence on their hydrogenation properties.

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