Electronic and electrochemical properties of Mg_2Ni alloy doped by Pd atoms

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Nanocrystalline metal hydrides are a new class of materials in which outstanding performance may be obtained by proper engineering of the microstructure. In this work, we study experimentally the structure and electrochemical properties of nanocrystalline Mg_2Ni phase modified by Pd impurities. Nanocrystalline Mg_2Ni - type alloys were prepared using mechanical alloying (MA) followed by annealing. The MA and annealed Mg_2Ni powder was mixed with 10 wt.% Pd powder and milled for 1h in a SPEX Mixer Mill. The weight ratio of hard steel balls to mixed powder was 30:1.

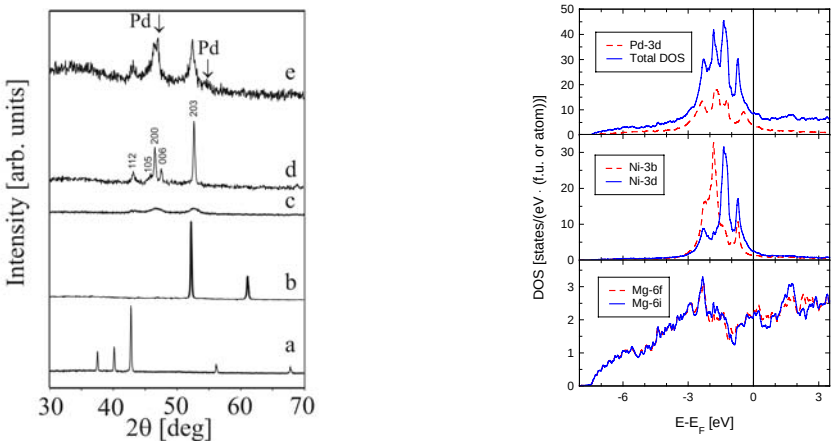

Fig. 1. X-ray diffraction patterns (Co-$K_{\alpha 1}$) of pure powders of magnesium (a) and nickel (b), and mixture of 2Mg and Ni powders after MA for 45 h (c) followed by annealing at 723 K for 1 h (d). Curve (e) represents XRD spectrum of Mg_2Ni/Pd composite prepared by MA for 1 h of nanocrystalline Mg_2Ni (see Fig. 1d) mixed with 10 wt.% Pd powder (left), total and site projected densities of electronic states (right).

The electronic structure was calculated using the FPLO® (version 5) method [1, 2] within coherent potential approximation (CPA) [3] to take into account chemical disorder introduced by Pd impurities. Above the densities of states are presented for the case when the Pd impurities are located in the *3d* site (Pd 10% and Ni 90%).

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[3] K. Koepernik, B. Velicky, R. Hayn and H. Eschrig, Phys. Rev. B **55** (1997) 5717

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