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Hydrogen diffusion through the Pd/Mg interface of Pd nanoparticles deposited on Mg nanofilms

Th. Pavloudis[1], S. Kumar[2], P. Grammatikopoulos[2], J. Kioseoglou[1], B. Clemens[3], M. Sowwan[2]
[1]*Physics Department, Aristotle University of Thessaloniki, GR-54124 Thessaloniki, Greece*
[2]*Nanoparticles by Design Unit, Okinawa Institute of Science and Technology Graduate University, 1919-1 Tancha, Onna-Son, Okinawa, 904-0495, Japan*
[3]*Department of Materials Science and Engineering, Stanford University, Stanford, CA 94305-4045, USA*

Abstract: Metal hydrides are a promising material for hydrogen storage, given their relatively low cost, abundance and high weight percent hydrogen absorption (e.g. 7.6 wt. % for magnesium hydride). However, to date, commercial application of metal hydrides has been limited by the relatively slow absorption and desorption kinetics, requiring high pressure and high temperature, respectively. A first approach for enhancing the properties of metal hydrides is nanostructuring, with the associated increase in surface area and reactivity that this inherently creates. Pd nanoparticles on Mg nanofilms may increase the efficiency of bulk Mg and offer an attractive alternative to bulk Pd for catalysis and hydrogen storage.
In this work, the diffusion of H in Mg nanofilms decorated with Pd nanoparticles is investigated by DFT using the VASP ab initio simulation package. Models of Pd and PdH on Mg and MgO are constructed and carefully relaxed and the specific reconstructions of the nanoparticle/nanofilm interface arising from the strain are examined. A single H atom is placed in a series of positions, starting from the nanoparticle region and ending deep in the nanofilm region and after the respective relaxations the diffusion path and energies are calculated and the diffusion barriers are extracted. The Pd nanoparticle is found to facilitate the diffusion of H in the first layers of Mg, significantly reducing the barrier compared to bulk Mg. This barrier is even smaller for PdH, suggesting that the diffusion is dependent on the H content of PdHx. Finally, H diffusion is not preferable in MgO for both Pd and PdH, suggesting that the nanofilm surfaces should not be oxidized before the nanoparticle deposition.