Hydrogenography: A combinatorial thin film approach to identify the thermodynamic properties metal hydrides

B. Dam
Condensed Matter Physics, Department of Physics and Astronomy, Faculty of Science, Vrije Universiteit, De Boelelaan 1081, NL-1081 HV Amsterdam, The Netherlands

The search for new light-weight metal-hydride storage materials is essentially that for a needle in a haystack. Although computational methods have become more and more realistic, their predictive power is still limited. Experimentally, the determination of the plateau pressures of bulk samples is a very time consuming proceure. This explains the renewed interest in high-throughput experimental methods. We demonstrate that the change in optical properties on hydrogenation make metal hydrides perfectly suited for a thin film combinatorial search for new hydrogen storage materials. Using Hydrogenography, we measure simultaneously the enthalpy of hydride formation of thousands of materials on a single thin film wafer. From extrapolation of the optically measured Van 't Hoff plots, we obtain the entropy of formation. In the ternary Mg-Ti-Ni phase diagram we demonstrate the destabilizing effect of Ti dopants on Mg_2Ni-hydride. Furthermore, we identify a composition region of Mg-rich Mg-Ti-Ni alloys that absorb hydrogen with enthalpies of formation between -40 and -37 kJ/(mol H_2). Using very thin layers of Pd we reproduce the Van 't Hoff relation both in absorption and desorption, fully in accordance with previous literature data. This shows that the technique is not limited to systems with a metal insulator transition. Since the chemisorption of hydrogen will always lead to some change in electronic structure, we think that our method is generally applicable.