Local structure of destabilised Mg-based alloys for hydrogen storage

Recently we started making Mg-based 3D nanostructured supported compounds in powder form. These compounds are formed by deposition of nanometer-sized particles (Ni) on a carbon support combined with magnesium melt-infiltration. These compounds show intriguing hydrogen sorption properties, but XRD analysis is not sufficient due to the lack of long range order. Our research has shown that EXAFS/XANES is a powerful tool to analyze nanoscale hydrogen storage materials, both in powder and thin film form. Studying the Ni local environments in Mg-based nanostructured compounds will reveal the structure of the phases present in the metallic and hydrogenated states, and will provide a substantial insight into the destabilization mechanism of the dopants.

We have performed transmission EXAFS and XANES measurements at the Ni K-edge on nanoscale Mg2-xNix/C powder samples (as-prepared and in the hydride form) (a) the metallic state (b) during and after hydrogenation by exposure to H2 and H2/He gas mixtures and (c) after de-hydrogenation by exposure to O2/He gas mixtures. Powder samples are prepared in a glove box with low water and oxygen levels, of the chemistry laboratory. Transmission scans are recorded for relevant powdered bulk and thin film reference systems.

We characterize the nanoscale structure present in the Mg2Nix/C samples. Mg2Ni(H4) and MgNi2(H4) are known compounds.

Preliminary, we have seen differences in the samples under study, as compared to the standard materials. Also, we have done in-situ de-hydrogenation and hydrogenation experiments on 7 differently prepared samples, giving interesting results. However, we will have to interpret the results with careful comparison and theoretical calculations. As these materials are new and the results are of high quality, we expect to publish this research in a high ranking journal soon.