In-situ investigation of deuterium sorption mechanisms in forged Mg-Mg_2Ni composites

Jing Wen[a,b], Thierry Grosdidier[b,c], Nathalie Allain[b,c], Marc Novelli[b,c] , Laetitia Laversenne[a], Patricia deRango[a]

[a]Université Grenoble Alpes, CNRS, Institut Néel, 38000 Grenoble, France

[b]Laboratoire d'Excellence Design des Alliages Métalliques pour Allègement des Structures, Université de Lorraine, France

[c] Université de Lorraine, CNRS, Arts et Métiers ParisTech, LEM3, F-57000 Metz, France

In the search for new materials for hydrogen storage, we investigate low cost Mg-Mg_2Ni composite materials. Samples processed by annealing and fast forging show a particular microstructure and a remarkable improvement of the hydrogen sorption kinetics.

In situ neutron diffraction was performed on CRG- D1b (ILL, Grenoble) to investigate the deuterium sorption mechanisms in Mg-Mg_2Ni composite materials. Neutron powder diffraction patterns were collected upon successive absorptions and desorptions while monitoring the deuterium pressure.

The sequence of phase transition for the first deuteration is very different from the subsequent ones. Upon the first deuteration (initial activation), deuterium evolution proceeds through the instantaneous formation of the solid solution $Mg_2NiD_{0.3}$ followed by almost simultaneously formation of the two deuteride phases MgD_2 and Mg_2NiD_4. The rate-limiting step for the first deuterium uptake is considered to be surface nucleation of the deuterides. Upon the second/third deuteration, a two-stage deuterium uptake accompanied by the sequential formation of deuterides occurred, where only the MgD_2 was formed during the first 17 min due to favorable thermodynamics and kinetics. Mg_2NiD_4 started to form once the formation of MgD_2 became gradually saturated.

We will show how *in situ* neutron powder diffraction coupled with sorption measurements and combined to kinetics analysis and microstructure observations uncover the sorption mechanisms in promising Mg-Mg_2Ni composite materials.