

Magnesium Nanoparticles for Hydrogen Storage: Structure, Kinetics and Thermodynamics

Luca Pasquini¹, Federico Boscherini¹, Amelia Montone², Marco Vittori Antisari², Ennio Bonetti¹

¹ Department of Physics and CNISM, University of Bologna, Italy

² ENEA, C.R. Casaccia, Rome, Italy

e-mail: luca.pasquini@unibo.it

The widespread interest in novel light-element solid-state hydrogen (H) storage media has triggered the investigation of a quite impressively variety of candidate materials. In alternative to the synthesis of new compounds, an interesting strategy consists in the engineering of nanostructures with a large specific area of properly functionalized surfaces. Nanoparticles (NPs) of light metal hydrides are appealing in this sense because their fine size and large surface area can lead to radically improved H-sorption kinetics. Moreover, the possibility that surface and/or interface effects alter the thermodynamics of the H-metal interaction could pave the way towards tunable hydride forming materials.

In this work we focus on magnesium-based NPs with metal/oxide core/shell morphology, synthesized by inert gas condensation and surface decorated by *in situ* post-evaporation of transition metal clusters [1-6]. The structure and morphology of the NPs are characterized by electron microscopy, including high-resolution observations. The kinetics and thermodynamics of H-sorption are investigated using standard laboratory techniques as well as *in situ* experiments of X-ray diffraction and absorption, that allow a correlation with ongoing structural transformations. In this respect we address several features like the irreversible formation of intermetallic phases, the H-induced reversible transition between these phases, and the possible formation of hollow nanoparticles driven by hydrogenation at sufficiently high temperature.

References

1. L. Pasquini et al., Appl. Phys. Lett. **94**, 041918 (2009)
2. E. Callini, L. Pasquini, E. Piscopiello, A. Montone, M. Vittori Antisari, E. Bonetti., Appl. Phys. Lett. **94**, 221905 (2009)
3. E. Callini, L. Pasquini, L.H. Rude, T.K. Nielsen, T.R. Jensen, E. Bonetti, J. Appl. Phys. **108**, 073513 (2010)
4. L. Pasquini et al., Phys. Rev. B **83**, 184111 (2011)
5. L. Pasquini, A. Montone, E. Callini, M. Vittori Antisari, E. Bonetti., Appl. Phys. Lett. **99**, 021911 (2011)
6. L. Pasquini et al., J. Nanopart. Res. **13**, 5727 (2011)