Some examples of in-situ diffraction measurements applied to the study of complex solid state hydrogen storage materials

Francesco Dolci

European Commission - JRC Institute for Energy, Petten, The Netherlands
E-mail: francesco.dolci@ec.europa.eu

The increasing worldwide concern for the effects of a growing atmospheric pollution on both climate and human health, is urging for a drastic change in energy policies. One of the most attractive suggestions for an efficient and clean energy carrier is hydrogen. Solid state hydrogen storage materials are considered as a possible alternative to gaseous or liquid hydrogen, since they combine high volumetric storage capacity together with a relative safety.

Among solid state storage options, complex hydrides aroused great interest for solid hydrogen storage applications as evidenced by the large number of experimental and theoretical works on this topic [1]. Recently the idea of mixing different complex hydrides together, or with light metal hydrides, has shown promising results and opened new possibilities for the design of practical hydrogen storage materials useful for both stationary and automotive applications. Results obtained by following this approach are however different from the ones expected on the basis of a simple thermodynamic modelling of the system. The main difference between the expected simple reaction pathway and the actual one is the presence of a multistep hydrogenation/dehydrogenation reaction. The lack of basic knowledge on the de/hydriding processes governing the behaviour of the mixture and sometimes of the single components themselves, hampers the development of new strategies for circumventing the limitations of the system and improving its performances.

In situ diffraction techniques above all, offer the unique opportunity of probing in real time and under experimental conditions the behaviour of the investigated compounds. Especially in-situ neutron diffraction seems to be a preferential choice for the study of hydrogen storage materials, since hydrogen is clearly identified and the structural characterisation of the compound can be complete and effective. Phase evolution during hydrogen absorption and desorption cycles and detection of new intermediate phases can be successfully pursued with a considerable improvement in the basic understanding of the material.

1. S. I. Orimo, Y. Nakamori, J. R. Eliseo, A. Zuttel and C. M. Jensen, *Chem. Rev.*, **2007**, 107, 4111-4132.