MS62.O01

Study of hydrogen storage materials by neutron powder diffraction

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Metal hydrides are interesting materials from a fundamental as well as practical point of view. Hydrogen storage applications have been the main driving force of research on these materials but lately uses such as thermal storage are considered. In this presentation we will review the use of neutron diffraction for the development of new metal hydrides. Two systems will be presented: BCC solid solution alloys and FeTi alloy. Ti-based BCC solid solutions are promising material for hydrogen storage applications which need high volumetric capacity and room temperature operation. One system that has been considered is Ti-V-Cr. Using only X-ray diffraction for structural identification does not provide information about hydrogen localization. Therefore, neutron diffraction is essential for complete determination of this class of hydrides. We will present examples of Ti-V-Cr compounds doped with Zr-Ni alloy. The peculiarity of this type of alloy is that, for neutron diffraction, the scattering lengths of the elements almost cancel. Therefore, the neutron pattern of as-cast alloy shows very small Bragg peaks but the advantage is that the hydride for is very easy to see and analyze. Another good candidate for hydrogen storage applications is the intermetallic compound TiFe which operates at around room temperature (RT) under mild pressure conditions. However one disadvantage of TiFe alloy synthesized by conventional metallurgical method is its poor activation characteristics. The alloy reacts with hydrogen only after complicated activation procedure involving exposure to high temperature (~400° C) and high pressure for several days. Recently we found that by doping this alloy with Zr and Zr7Ni10 the activation could be easily done at room temperature. We present here a neutron diffraction study of these compounds that shows the structural difference between the activated compound and the one cycled under hydrogen.

Keywords: Metal hydrides, neutron, structure refinement