In-situ / Ex-situ Neutron Diffraction Investigation of Ti-V-Mn alloys and its Deuterides

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For the development of a future hydrogen economy practical ways to store hydrogen have to be established. Metal hydrides with their high volumetric capacities (higher than liquid hydrogen) could be used for some specific applications that need compact and safe way to store hydrogen. Recently we found that in the Ti-V-Mn and Ti-FeV-Mn systems upon hydrogenation two different hydrides phases are formed [1]. From X-ray powder diffraction it was found that $Ti(FeV)_{1.2}Mn_{0.8}$ alloy crystallize in a C14 + BCC multiphase system. Upon hydrogenation, contrary to what should be expected, the lattice parameters of both phases increase without formation of a FCC structure. Neutron powder diffraction will help us understand the effect of hydrogenation on the crystal structure of this alloy. Two specific compositions $TiV_{1.2}Mn_{0.8}$ and $Ti(FeV)_{1.2}Mn_{0.8}$ were investigated in-situ using a newly developed system which enables to perform pressure-composition-temperature (PCT) measurements simultaneously with NPD measurements. Figure 1 shows the neutron diffraction pattern of $Ti(FeV)_{1.2}Mn_{0.8}$ taken at different deuterium loadings. It confirms that upon hydrogen loading the crystal structure is unchanged and lattice parameters increases. However, neutron patterns will enables us to precisely locate the deuterium atoms in both structures and to measure the impact of hydrogenation on the thermal parameters. This analysis is presently under way.

Reference

[1] M. Tousignant, J. Huot, Replacement of vanadium by ferrovanadium in Ti-based BCC alloys for hydrogen storage, *Solid State Phenomena*, Vol. 170 (2011), p 144-149

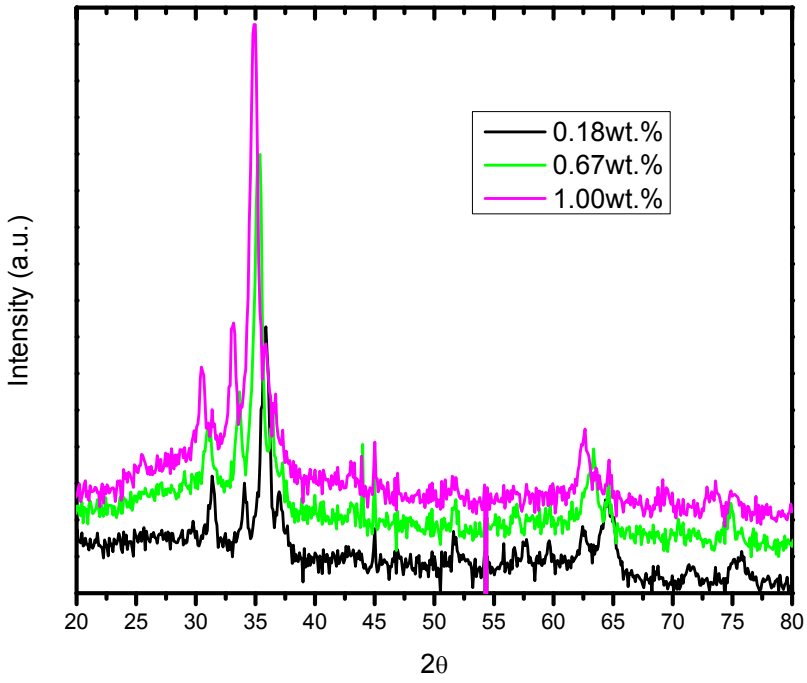

Fig. 1 Neutron diffraction patterns of $Ti(FeV)_{1.2}Mn_{0.8}$ at different hydrogen loadings (in wt.%).