Reversibility of solid-gas and electochemical hydrogenation of Ti-based AB-type alloys studied by in-situ neutron diffraction

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Most metals can react with hydrogen to form either very stable or unstable metal hydrides. First ones, classed as *A*-type, comprise alkali, alkali-earth, rare earth and early transition metals. Their hydrides need to be heated well above room temperature to desorb hydrogen near atmospheric pressure. Second ones, classed as *B*-type, are late transition metals and *p*-type elements. Their hydrides are only formed at hyperbaric pressures well-above 100 atm. The association of *A* and *B*-type metals to form AB_n intermetallics allows reversible hydrogen storage at normal conditions of pressure and temperature [1].

Ti-based *AB* intermetallics are remarkable materials for hydrogen storage as they are so far the best compromise between capacity and reversible loading at room temperature while keeping affordable cost. The association between *A*-type titanium metal and *B*-type late transition 3*d* metals such as Fe, Co and Ni offers not only the possibility to store large amounts of hydrogen but also to tune, through chemical substitutions, their thermodynamic properties [2]. Disregarding the remarkable exception of TiNi that exhibits polymorphism and shape memory properties, all Ti-based *AB* intermetallics crystallize in the cubic CsCl-type structure [3].

In this presentation, hydrogenation properties of Ti*B*-type intermetallics (*B* = Fe, Co and Ni) will be reviewed with focus on the Ti(Fe,Mn) and Ti(Ni,Cu) systems and their application for large-scale solid-gas hydrogen storage [4] and as negative electrodes of Ni-*M*H batteries [5], respectively. The use of in-situ neutron diffraction to unveil hydrogenation mechanisms [6], as shown in Figure 1 for the Ti(Fe,Mn) system [7], will be particularly highlighted.

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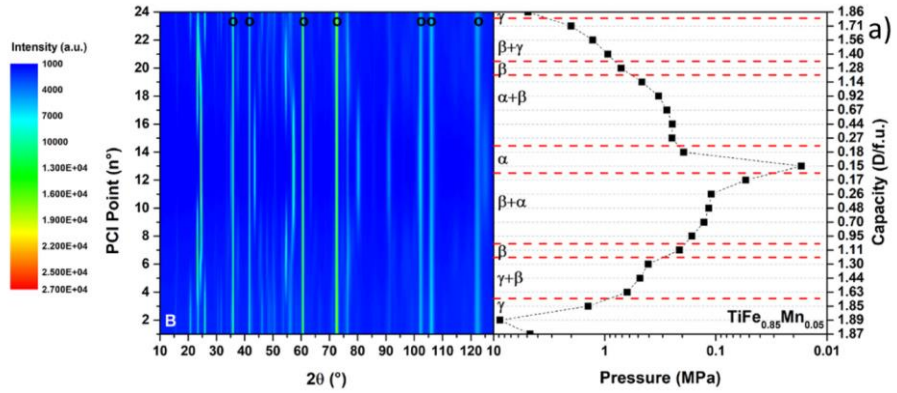

Figure 1: In situ neutron diffraction 2D patterns (counter plot, λ = 1.286 Å) and PCI curve at RT during deuterium desorption /absorption between 0.02 and 9 MPa for $TiFe_{0.85}Mn_{0.05}$ alloy.

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