Synchrotron X-ray techniques as a tool to investigate and design new materials for hydrogen storage

Guilherme Zepon

Abstract: Hydrogen plays a key role in the transition from an energy matrix based on fossil fuel to a matrix based on renewable and low-carbon sources. In this context, hydrogen acts as an energy vector in which the surplus energy produced by renewable sources is used for its production, through electrolysis or biomass reform, for example. The hydrogen produced can be stored, distributed, and converted back into useful energy through fuel cells or combustion engines. One of the major bottlenecks for the widespread use of hydrogen as an efficient energy carrier lies on its storage and transport, which is mainly limited by the low density of this gas even at high pressures. Solid-state hydrogen storage in metal hydrides is one of the most promising alternatives to solve this problem. In-situ synchrotron X-ray diffraction is an important tool to investigate the structural changes that takes place during hydrogenation/dehydrogenation reaction, which is paramount to allow materials scientists to tune the hydrogen storage properties of metal hydrides. In this work, it will be presented the application of in-situ synchrotron X-ray diffraction in the investigation of a series of Mg-based complex hydrides. In addition, it will also be presented the application of synchrotron radiation Pair Distribution Function (PDF) in the investigation of the local structure of body-centered cubic (BCC) multicomponent alloys of the Ti-V-Nb-Cr system. In the last decade, the interest on multicomponent alloys for hydrogen storage applications have been increasing since their hydrogen storage properties are very compositional dependent and, therefore, multicomponent systems give the possibility to design alloy compositions with optimized hydrogen storage properties for each specific application. The hydrogen storage properties of these alloys are very dependent on the local structure, i.e., on the local environment around the interstitial sites where hydrogen atoms are absorbed.

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