Invited talk at the Microsymposium “ENERGY STORAGE MATERIALS”

IN-SITU AND HIGH-RESOLUTION POWDER DIFFRACTION STUDIES OF COMPLEX METAL-HYDROGEN SYSTEMS

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In the first part of the talk I will focus on a combined characterization of metal-hydrogen systems by in-situ and high resolution powder diffraction both with neutrons and synchrotron radiation. HoNi$_3$-$\text{H}_2$ [1] and ErCo$_3$-$\text{H}_2$ [2] systems will be used to illustrate the power and potential of each method. In-situ studies provided information on the metal-hydrogen phase diagrams, while high resolution ex-situ diffraction revealed subtle structural features like symmetry lowering, changes in metal atom substructure, metal-hydrogen bonding. The Ni-containing system reveals at least three hydride phases, shows a hydrogen-induced transition from centro- to noncentrosymmetric space group (a challenge to detect by powder diffraction!) and ordered pyramidal [NiD$_3$] fragments. The Co-containing system demonstrates quite a different behaviour.

Finally I will present two difficult structures of metal hydrides solved from powder data. The first, Zr$_2$CuD$_{\sim5}$ [3], shows complete reconstruction of the metal matrix (near ambient conditions!), and therefore its structure had to be solved ab initio. The situation has been complicated by a huge intrinsic broadening of the diffraction lines and a low structure symmetry (monoclinic for the hydride versus tetragonal for the alloy). The second, Mg(BD$_4$)$_2$, is a very complex structure recently solved by direct space methods (program FOX) using synchrotron and neutron powder data.