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. $HoNi_3$-H_2 [1] and $ErCo_3$-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, $Zr_2CuD_{\sim 5}$ [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.

[1] Y. Filinchuk, D. Sheptyakov, K. Yvon, J. Alloys Comp., 413 (106-113), 2006
[2] Y. Filinchuk, K. Yvon, J. Solid State Chem., 179 (1041-1052), 2006
[3] Y. Filinchuk, K. Yvon, Inorg. Chem., 44 (8191-8193), 2005