Transition metal-based hydrides: combining *in-situ* and high-resolution neutron powder diffraction studies

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Abstract:
In this study we focused on those metal hydrides, which could be traditionally considered as "interstitial", but their structures appear to be highly influenced by transition metal-hydrogen (T-H) interaction. Each metal-hydrogen system has been studied first by *in-situ* NPD (DMC) under controlled deuterium pressure, and then the individual phases were studied *ex-situ* by high resolution NPD (HRPT). Each system revealed two to three hydride phases, stable at certain temperatures and pressures (deuterium concentrations). While the symmetry of a deuteride structure is usually lower than that of the corresponding alloy, a metal atom substructure may undergo a complete reconstruction upon hydrogenation. In some systems the T-H contacts appear to be short and directed (like in non-metallic complex transition metal hydrides), thus affecting a structure and properties of the hydride phases. In my talk these observations will be illustrated with the following systems:

- $HoNi_3$-D_2 [1]: three hydride phases; *R*-3*m* $\rightarrow$ *R*3*m* transition; ordered pyramidal [NiD_3] fragments;
- $ErCo_3$-D_2 [2]: two hydride phases; symmetry preserved; disordered octahedral [CoD_4] fragments;
- Zr_2Cu-D_2 : *I*4/*mmm* $\rightarrow$ *I*2/*m* and complete reconstruction of the metal matrix near ambient conditions! [3]; plus two other hydride structures at high temperatures;
- La_3Pd_5Si-D_2 : three hydride phases; different Pd-D fragments; a method was developed to characterize hydrides with very high equilibrium pressure.

In-situ synchrotron diffraction at SLS and SNBL (ESRF) will also be discussed.

References:
[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

SINQ instruments involved:
HRPT, DMC