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EXAFS INVESTIGATIONS ON NOVEL LAVES PHASE HYDRIDES

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The Laves phases are interesting materials for future hydrogen energy development. They represent a group of intermetallic compounds that, besides of very interesting physical and chemical properties, are considered as important hydrogen storage materials. Generally, they are stable for a long time at normal conditions [1]. Recently a number of novel hydrides/deuterides materials were synthesized by treating various Laves compounds under high hydrogen/deuterium pressure. The most interesting is the group of YMn_2D_6 complex deuterides doped with Cr or Fe.

Although their properties were intensively investigated, the position of Mn and Cr/Fe atoms in the crystal structure and electronic structure of these compounds is not completely clear yet.

Submitting YMn_2 to high hydrogen pressure leads to the formation of a novel, unique YMn_2D_6 deuteride with *Fm*-3*m* symmetry (see Fig. 1) [2]. The YMn_2D_6 was synthesized for the first time by submitting YMn_2 to deuterium at 1.7 kbar pressure at 473 K. According to X-ray (XRD) and Neutron Powder Diffraction (NPD) experiments, YMn_2D_6 crystallizes in the K_2PtCl_6 – type cubic structure with a = 6.709(1) Å at 300 K. The Y and half of the Mn atoms occupy the *8c* site whereas the other Mn atoms are located in *4a* site and are surrounded by 6 D atoms (*24e*). The Mn(*4a*)-D distances are around 1.65 Å [2].

Investigated materials were synthesized at the Institute of Physical Chemistry PAS in Warsaw in collaboration with French and Taiwanese Partners. Among obtained materials especially interesting is the group of YMn_2D_6 complex deuterides additionally doped with Cr or Fe atoms.

Despite large number of reports about properties of Laves hydrides, there is not much reported about structural changes under high pressure especially local atomic structure around Cr or Fe dopants.

The X-ray Absorption Spectroscopy (XAS) offers unique possibility to localize the position of atoms inside the crystal structure and to estimate the chemical bonding of elements as well as changes introduced by different treatments. Therefore, it is an ideal tool for study these novel hydrides of Laves phase.

EXAFS measurements of Mn, Cr and Fe K edge were preformed at Hasylab at E4 station. Transmission and fluorescence modes of detection at LN temperature were used. Samples were powders and were prepared under Ar atmosphere in order to avoid oxidation.

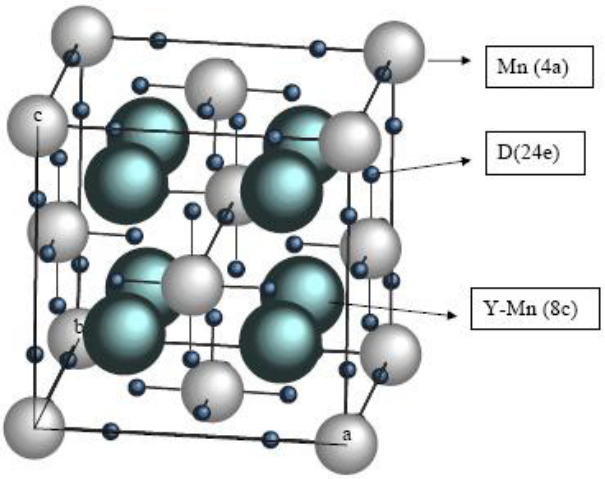

Figure 1. Crystal structure of YMn_2D_6 in *Fm*-3*m* space group.

EXAFS data analysis confirmed change of YMn_2 crystal structure after deuteration (see Fig. 2). Moreover, two equivalent positions of Mn atoms in YMn_2D_6 were also identified [Mn (0, 0, 0) and Mn (¼, ¼, ¼)].

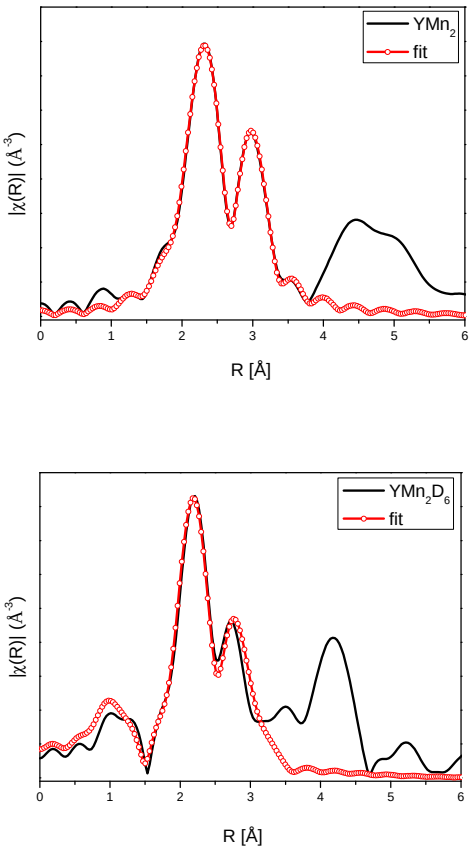

Figure 2. Fourier transformed experimental EXAFS spectra, for Mn K-edge, together with fitting result for YMn_2 and YMn_2D_6.

Furthermore, Mn K edge investigation indicated that addition of Cr atoms up to 10% did not change distribution of Mn between two equivalent positions in the lattice. However, when 20% of Cr atoms is incorporated then 90% of Mn were found in the (¼, ¼, ¼) position (see Fig. 3).

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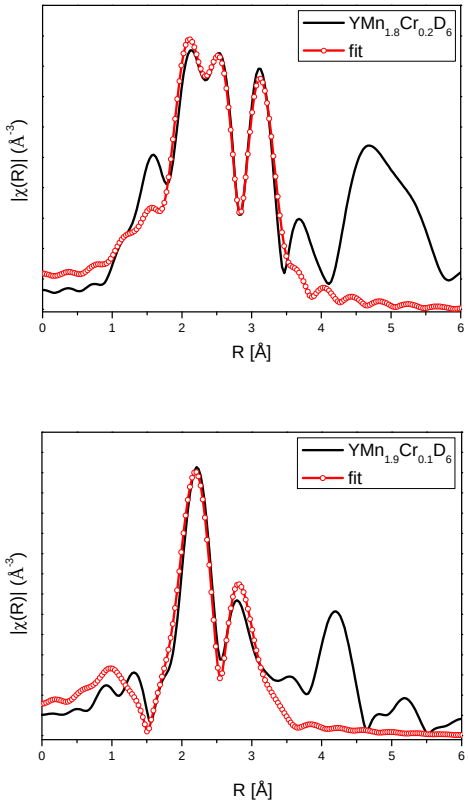

Figure 3. Fourier transformed experimental EXAFS spectra, for Mn K-edge, together with fitting result for $YMn_{1.8}Cr_{0.2}D_6$ and $YMn_{1.9}Cr_{0.1}D_6$.

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