SNBL experiment report

Dates of experiments: 04 February 1999 (7:00) - 08 February 1999 (07:00)
Experiment # 01-01-164
Beamline: BM01B

Experiment title:

STUDIES OF CRYSTAL STRUCTURES OF INTERMETALLIC HYDRIDES AND H-INDUCED PHASE TRANSFORMATIONS BY MEANS OF HIGH RESOLUTION POWDER DIFFRACTION

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This project was aimed on studies of the Hydrogenation-Disproportionation-Desorption-Recombination (HDDR) process which plays a significant role in the processing of a new generation of the rare earth containing permanent magnets and hydrogen storage alloys. A particular emphasis was focused on the behaviours of oxygen-doped zirconium-containing intermetallics, possessing advanced H-storage characteristics, and, also, on studies of H behaviour in the $Nd_5Co_2B_6$ intermetallic compound, a possible constituent of the Co-doped NdFeB magnets with increased energy product.

Main results:
A scheme of hydrogen disproportionation process was established for the Zr_4Fe_2O mixed oxide. It can be presented by the following equation:

$$2\ Zr_4Fe_2O + 5\ D_2 \rightarrow \quad 5\ \varepsilon\text{–}ZrD_2 + 2\ ZrFe_2 + ZrO_2$$

A complete recovery of the original Zr_4Fe_2O structure proceeds on deuterium desorption indicating a diffusion of oxygen between the coexisting phases in presence of hydrogen instead of a recovery of the oxides. This keeps a constant O content in the metal matrix.

A formation of a new, previously not known binary boride NdB_2 has been confirmed from the analysis of the data for the disproportionated (in deuterium) $Nd_5Co_2B_6$ boride. NdB_2 has the following crystallographic characteristics: AlB_2 structure type; space group P6/mmm; a = 3.3064(5); c = 3.8427(9) Å.

Finally, a phase diagram of the system Zr_2Ni-D_2 has been studied in a wide range of D compositions, in relation to the P-T conditions employed to synthesise the deuterides.

The results of the evaluation of the experimental data collected by our group at SNBL in 1998 have been published in the following papers:

V.A.Yartys, H.Fjellvåg, I.R.Harris, B.C.Hauback, A.B.Riabov, M.H.Sørby, I.Yu.Zavaliy. H-induced phase transformations and hydrogen ordering in Zr-based intermetallic hydrides.// *J.Alloys and Compounds*, 293-295 (1999), 74-87.

B.C.Hauback, H.Fjellvåg, L.Pålhaugen, V.A.Yartys, K.Yvon. Crystal and magnetic structure of $TbNiAlD_{0.3}$ studied by neutron diffraction and synchrotron radiation.// *J.Alloys and Compounds*, 293-295 (1999), 178-184.