STRUCTURAL CHARACTERIZATION OF METAL HYDRIDES USING DIFFRACTION METHODS

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Detailed knowledge about the positions of the atoms is of major importance both for development of new compounds and for understanding of their properties. Neutron diffraction is a unique tool for studies of metal hydrides since it is the only method to determine the positions of the hydrogen/deuterium atoms in the crystal structures. For structural studies the use of deuterium is crucial due to the challenge with incoherent scattering with normal hydrogen (protium). For studies of boron-based compounds, borohydrides, the ^{11}B isotope has to be used because of the strong absorption of neutrons in normal boron (mainly ^{10}B). Furthermore, the weak interaction of neutrons with most elements results in determination of real bulk properties and easy use of complex sample environments. Most of our powder neutron diffraction (PND) experiments are performed with the high-resolution powder diffractometer PUS at the JEEP II reactor at IFE.

For studies of complex structures and samples containing different phases, the combination of PND and X-ray diffraction is needed. For very complicated structural features and *in-situ* experiments, the use of synchrotron radiation powder X-ray diffraction (SR-PXD) is important. SR-PXD is in particular important for detailed studies of hydrogen absorption and desorption where presence of crystalline phases during the sorption processes can be determined. Our SR-PXD experiments are performed at the Swiss-Norwegian Beamlines (SNBL, BM01) at the ESRF, Grenoble, France. Small-angle neutron scattering (SANS) at IFE combined with SAXS at ESRF gives information about size and shape of nanoconfined metal hydrides.

Selected detailed structural studies and *in-situ* sorption diffraction experiments will be presented. The presentation will address recent studies of metal hydrides and in particular borohydrides and other complex hydrides. Selected examples of novel compounds, efforts to understand hydrogenation/dehydrogenation properties including effect of selected additives, will be described. The combination of neutron and synchrotron radiation X-ray scattering is in particular important and will be emphasized.

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