7 Hydrogen Project

– Observation of the quantum nature of hydrogen in materials –

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7-1 Hydrogen project meeting

Quantum beams such as neutron, X-ray and muon beams are expected to be useful for observing the position of hydrogen, bonding of hydrogen with surrounding atoms, and so on. However, none of these beams can observe the entire nature of hydrogen in materials: a neutron beam can observe the proton of hydrogen but not electrons, an X-ray beam can observe electrons but not protons, and a muon beam can observe the excitation state of hydrogen but not muon-trapped sites. This project brings together specialists in neutron, synchrotron and muon beams for observing hydrogen and aims to clarify the quantum nature of hydrogen in materials through the exchange of information on state-of-the-art techniques and projects with external funds. The first meeting of the hydrogen project was held on September 13th at KEK. The program is as follows.

"Observation of hydrogens in matter with quantum beam techniques"

Overview of the CMRC hydrogen project
T. Otomo (KEK)
Structural studies of metallic hydride under high-pressure
A. Machida (JAEA)
Frontiers of soft X-ray emission spectroscopy: operand spectroscopy
Y. Harada (ISSP, U. Tokyo)
Isotope effects of hydrogen in Mg_2FeH_6 with soft X-ray inelastic scattering
D. Sekiba (Tsukuba U.)
Neutron quasi-elastic scattering of hydrogen storage systems
O. Yamamuro (ISSP, U. Tokyo)
Structural studies of light-metal hydrides
K. Ikeda (KEK)
Comments on materials development
S. Orimo (Tohoku U.)

Fig. 1: Photograph of the hydrogen project meeting

7-2 Local structure analysis of hydrogen storage materials

$NaAlH_4$ is a promising hydrogen storage material. The hydrogen release rate of $NaAlH_4$ is increased ten-fold by adding a few mol% of Ti. This reaction is a solid-state disproportional reaction and is reversible (Fig. 2). Hydrogen defects are thought to be closely related to the reaction but the mechanism of the reaction has not been revealed from the atomic structural point of view.

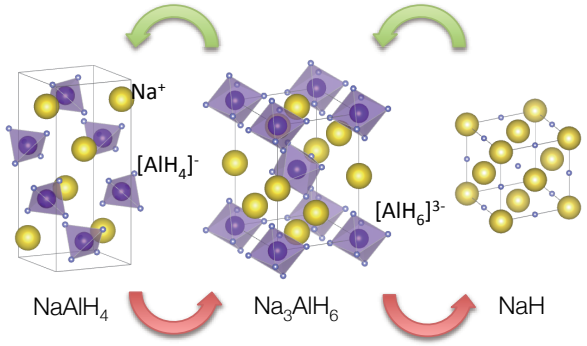

Fig. 2: Reversible hydrogen absorption and desorption reaction of $NaAlH_4$.

The hydrogen absorption and desorption processes of $NaAlH_4$ are being investigated by complementary usage of neutrons and X-rays. Neutron total scattering studies involving in-situ measurement of the hydrogen absorption and desorption processes are being conducted at J-PARC to analyze diffuse scattering intensity and obtain information on hydrogen defects. XAFS measurements of Al and Ti K-edges have been performed at the KEK PF. The local structure of Al-H units will be analyzed by combining neutron diffraction and XAFS results.