7 Hydrogen Project

– Observation of the quantum nature of hydrogen in materials –

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7-1 Structural study of Pd-D nano-particle by neutron scattering

The synthesis of nano-particles of metals is interesting for developing catalysts and basic properties by size and surface effects. There have been many reports that hydrogenation and hydrogen diffusion in nano-particles of metals are different from those in bulk metals. Pd-H shows anomalous heat capacity at 50 K. In contrast, nano-particle Pd-H shows a different temperature behavior of heat capacity, suggesting that tunneling diffusion of hydrogen occurs in the nano-particle Pd-H. In order to investigate the atomic position of hydrogen in Pd nano-particles, D_2 gas in-situ measurements were performed on the high-intensity total diffractometer, NOVA, at J-PARC.

Figure 1 shows the diffraction profile of nano-particle $PdD_{0.363}$ (average diameter is about 8 nm). Results of Rietveld refinement suggest that tetrahedral hydrogen sites, in which four Pd atoms are coordinated around a hydrogen atom, were occupied by hydrogen as well as octahedral hydrogen sites, in which six Pd atoms are coordinated around a hydrogen atom. This is in contrast to bulk Pd because only octahedral sites are occupied in the fcc structure of the bulk state. This site occupancy may relate to the diffusion behavior of hydrogen in the nano-particle. Further investigations are ongoing.

(H. Akiba, M. Kofu, O. Yamamuro, H. Kobayashi, H. Kitagawa, K. Ikeda and T. Otomo)

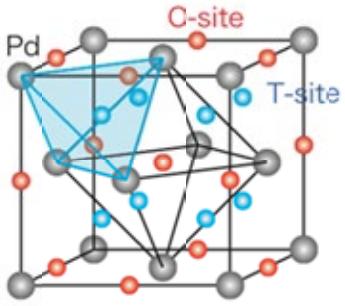

Fig. 1: Octahedral site (O-site) and tetrahedral site (T-site) in fcc structure.

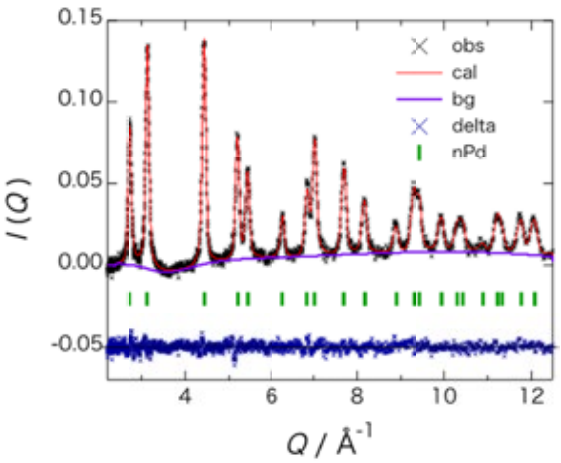

Fig. 2: Results of Rietveld refinement of $PdD_{0.363}$ nano-particle.

7-2 Catalytic effect of a hydrogen storage material, $NaAlH_4$

$NaAlH_4$ is a promising material for storing hydrogen. The hydrogen release rate of $NaAlH_4$ is increased ten-fold by the addition of a few mol% of Ti. This reaction is a solid-state disproportional reaction and is reversible (Fig. 3). It is expected that hydrogen defects are closely related to the reaction but the mechanism of the reaction has not

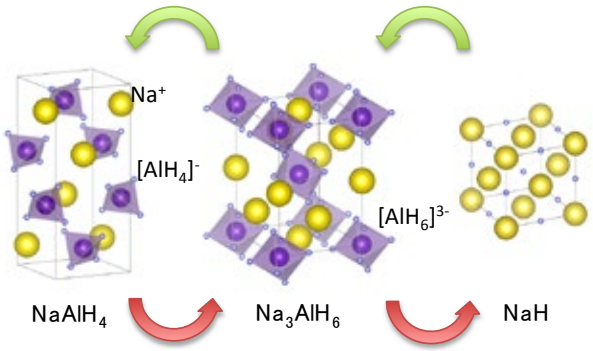

Fig. 3: Reversible hydrogen absorption and desorption reaction of $NaAlH_4$.

been revealed from the atomic structural point of view.

The addition of Ti is the key to achieving a reversible reaction. XAFS measurements and anomalous X-ray scattering (AXS) around the Ti K-edge have been performed at the KEK PF. The results suggest that some of the Ti atoms are replaced with Al atoms in $NaAlH_4$ and that other forms of Al-Ti are allowed outside of $NaAlH_4$. AXS measurement of $NaAlH_4$ was performed for the first time in $NaAlH_4$–Ti systems, and the replacement of Al atoms by Ti was revealed.