Hydrogen Dynamics in Pd Nanoparticles

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Hydrogen diffusion in metals is classified as the fastest atomic diffusion in solids and it is also well known that nanometer-sized metal shows particular properties, which depend on the particle size. Motional properties of hydrogen in the metal nanoparticles, hence, are expected to exhibit somewhat exotic behavior. Especially, we are interested in the quantum mechanical motion of hydrogen, \textit{i.e.}, tunneling diffusion. Here, we will show an indication of such a motion in the study on dynamics of hydrogen absorbed in the polymer-coated Pd nanoparticles.

\textsuperscript{2}H NMR spin-lattice relaxation times ($T_1$) for deuteron atoms in the Pd nanoparticles showed a particular minimum below 30 K while $T_1$ for the bulk sample increase monotonously with decreasing temperature. The spin-lattice relaxation for bulk Pd follows Korringa relation, implying that the relaxation of deuteron atoms is brought by the transition of conduction electrons in. On the other hand, it is known that thermally activated diffusion of deuteron atoms, also causing spin-lattice relaxation, does not occur in Pd below 50 K. Therefore, tunneling diffusion of deuteron atoms in the nanoparticles might be an origin of the $T_1$ minima observed below 30 K.

Neutron scattering experiments were carried out for the bulk and nanoparticle of Pd hydrides (7.1 ± 1.4 nm) with AGNES spectrometer installed at JRR-3 (JAEA, Japan). AGNES is a chopper-type TOF spectrometer similar to IN6 at ILL. The wavelength of monochromated neutron is 4.22 Å and the corresponding energy resolution at elastic position is 120 micro-eV. The scattering intensity from absorbed hydrogen atoms was evaluated from the intensity difference between the samples with and without hydrogen atoms. The signals from the hydrogen atoms absorbed in bulk Pd and Pd nanoparticles are shown in Figs. 1(a) and (b), respectively. As for the bulk samples, the scattering intensity increased with increasing temperature. This is the contribution from phonons as expected from the inelastic neutron scattering data at much higher temperatures. On the other hand, the intensities for the nanoparticle sample, especially at around 1 meV, increased with decreasing temperature.

![Fig. 1. Neutron scattering from hydrogen absorbed in (a)Pd black and (b)Pd nanoparticle.](image-url)
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Recent Publications:

Biographical Sketch:
A research work on dynamics of hydrogen absorbed in metal nanoparticles by Associate Professor Yamauchi started in 2001 when she was a postdoctoral fellow in Department of Chemistry, University of Tsukuba. Since then she has been studying hydrogen storage in nanoparticles and relating topics for 8 years. In 2003, she became an assistant in Kyushu University. In 2008, she was promoted to an associate professor in Catalytic Research Center, Hokkaido University.