XAFS analysis of hydrogen storage material under H_2 gas flow condition

In order to achieve carbon-neutral and hydrogen-based society, it is increasingly desired to understand the material characteristics under hydrogen atmosphere. We will introduce an example in which the generation of palladium hydride from palladium metal was identified by H_2 flow *in situ* XAFS analysis.

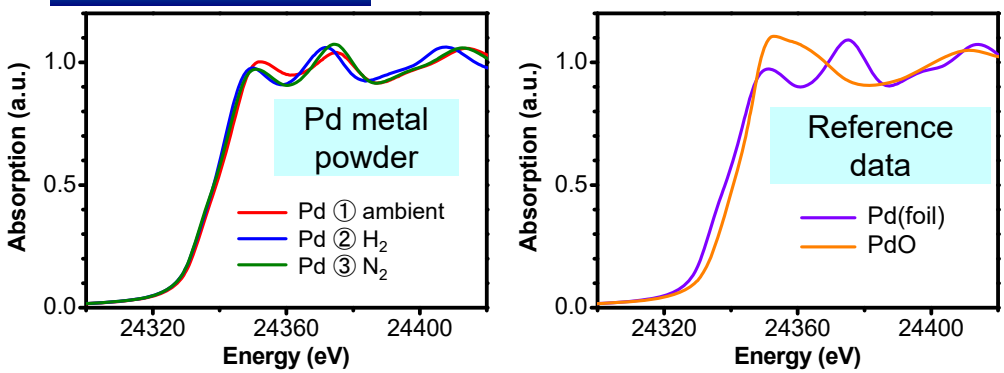
1. Sample, Experimental

sample：Palladium powder

① **ambient condition**
② **H_2 flow***
③ **N_2 flow***

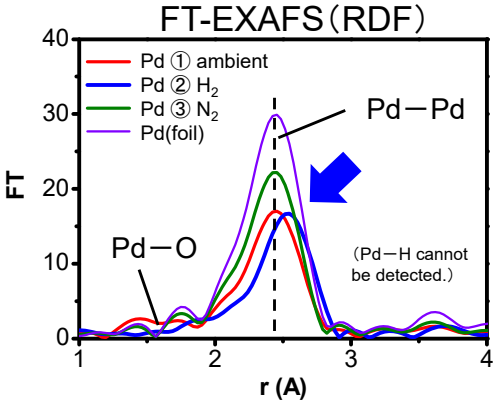
* under 100% H_2 or N_2, 100 cc/min. flow with gas flow *in situ* cell

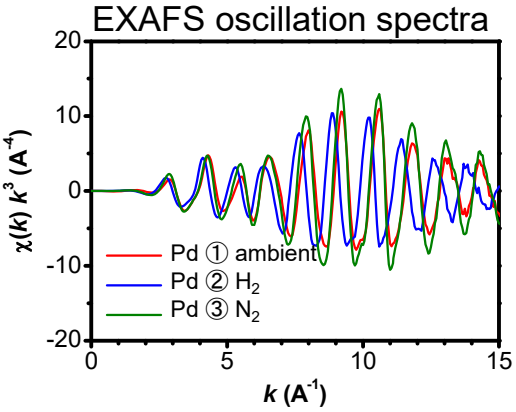
2. XANES spectra



①: Pd metal with Pd oxide was identified.
②, ③: Pd^0 was a main component in spite of the difference between ② and ③.
→ H_2 storage and Pd hydride generation was suggested.

3. FT-EXAFS, EXAFS oscillation spectra





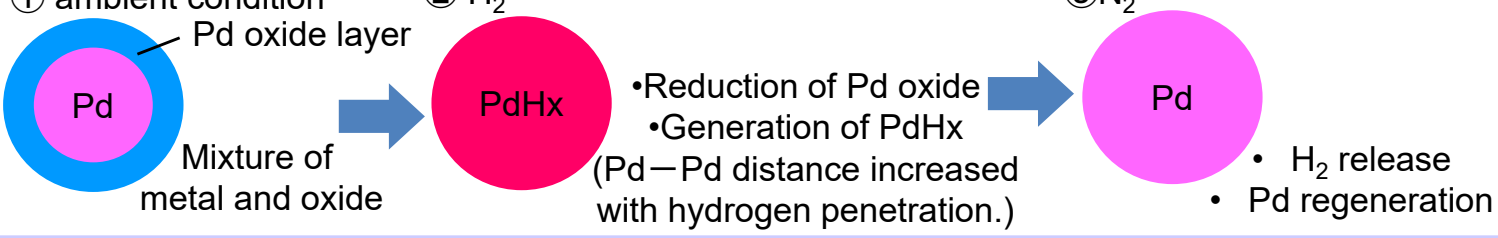
Pd－Pd bonding distance from EXAFS curve fitting

Pd－Pd	R (Å)
① ambient condition	2.74
② H_2	**2.83**
③ N_2	2.74

Ref） Pd-Pd distance (analyzed by diffraction)
Pd metal：2.75 Å, Pd hydride：2.84 Å(PdHx)

①, ③: The Pd－Pd bonding of normal palladium was detected.
②: The Pd－Pd distance increased with hydrogen penetration.

4. Schematic image of state and structural transition of Pd



Toray Research Center has a menu of evaluation under hydrogen by gas-flow *in-situ* analysis and hydrogen pretreatment !

Toray Research Center, Inc.