Wilde研究室

[Atomic Level Near-Surface Hydrogen Dynamics]

Department of Fundamental Engineering

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Nanoscale Surface Physical Chemistry

Graduate School of Engineering, Department of Applied Physics

Elucidating Hydrogen Absorption & Recombination

Nanoscale Analysis of Hydrogen Distribution, Diffusion, and Reactions at Surfaces and Interfaces

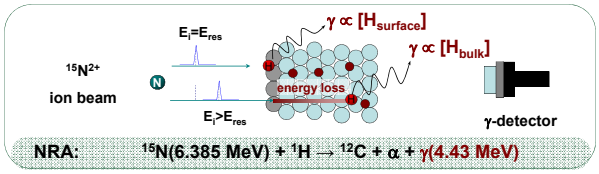
Near-surface absorbed hydrogen in platinum group metals has important applications in clean energy (H_2) storage, industrial hydrogenation, and fuel cell catalysis. The detailed microscopic pathways of reversible hydrogen transitions between the gas or liquid phase, the surface, and the interior of the metals, however, still remain mysterious even today. We therefore strive to understand hydrogen absorption and recombination dynamics at the atomic level using well-characterized single crystal surfaces. We further explore the peculiar H-storage behavior of nanoparticles and investigate the special catalytic reactivity of subsurface-absorbed hydrogen.

◆ Experimental Techniques

- ✓ *Nuclear Reaction Analysis (NRA)*: Non-destructive hydrogen depth profiling ・ Identification of *surface-adsorbed* and *'subsurface-absorbed'* H ・Real space visualization of H-breathing by metallic nanocrystals
- ✓ *Thermal Desorption Spectroscopy (TDS)*: Thermal stability of hydrogen species ・ Hydrogen absorption kinetics・Surface/subsurface-H exchange ・ Isotope effects in surface penetration and bulk diffusion
- ✓ *High Resolution Rutherford Backscattering (HRBS)*: Shape/size-assessment of nanostructures ・ Sub-nm (light) elemental depth profiling ・ Surface and ultra-thin film composition analysis

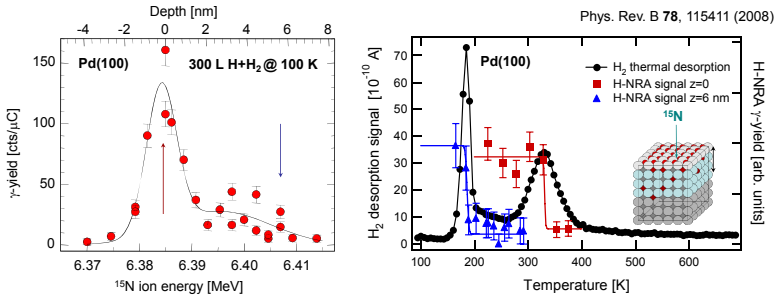
◆ Hot topics from latest research

- ✓ *Hydrogen storage* → H-Absorption/Release Mechanism
- ✓ *Hydrogenation Catalysis* → Reactivity of 'Subsurface-H'
- ✓ *MOS Devices* → Relation of H-Impurities and Reliability



On the Mechanism of H-Penetration/Recombination at a Pd Single Crystal Surface

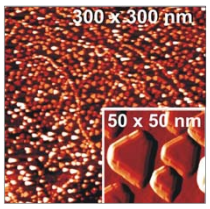
Phys. Rev. B **78**, 115411 (2008)



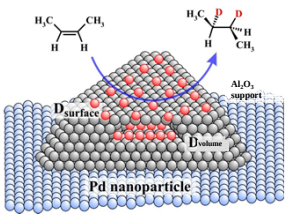
Surface-adsorbed H and *subsurface-absorbed* H species are identified by NRA and TDS.

On the Catalytic Role of Absorbed-H in Pd-Nanocrystals

Angew. Chem. Int. Ed. **47**, 9289 (2008); Phys. Rev. B **77**, 113412 (2008)

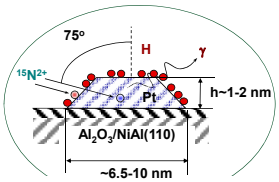


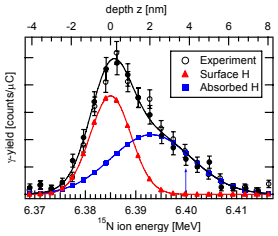
Oxide-supported Pd-Nanocrystals

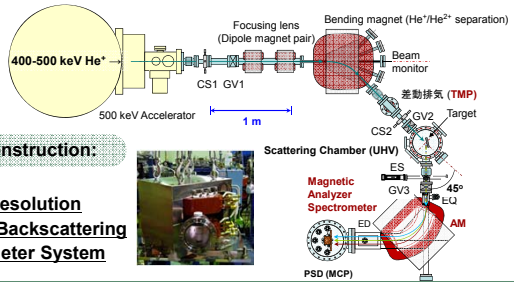


Model Hydrogenation Catalyst

First direct proof (NRA) for the involvement of **nanocrystal-absorbed hydrogen** in **olefin hydrogenation catalysis**.







Under Construction:

High Resolution Rutherford Backscattering Spectrometer System