CDCS
CENTER FOR DATA AND COMPUTING
IN NATURAL SCIENCES

OPENING SYMPOSIUM 2022

Universität Hamburg
DER FORSCHUNG | DER LEHRE | DER BILDUNG

DESY.

TUHH

Contribution ID: **92** Type: **Poster**

Dynamics of oxygen-induced shape changes of supported Palladium nanoparticles

Understanding the dynamics such as shape changes observed in oxidation and reduction reactions of metal nanoparticles remains elusive. These processes occur at higher temperatures and under gas exposure on ultrafast time scales of femtoseconds to nanoseconds, and are crucial for understanding of fundamental processes in heterogeneous catalytic reactions. Here we present a detailed study of the structural response of an ensemble of palladium nanoparticles around 10 nm in diameter supported on a MgO substrate upon laser excitation with 0.1 ps time resolution. The goal of this work is to investigate how the palladium nanoparticles'shape changes during oxygen desorption. The nanoparticle shape change is induced by desorbing the oxygen with a laser excitation and the X-ray diffraction signal is measured in a pump-probe manner.

Preliminary experiments were performed the Materials Imaging and Dynamics instrument at the European XFEL. Pump-probe delay scans with the Pd sample at room temperature and purged with Ar were measured at different laser power levels, 20, 40, 60, 80, 100% of the maximum pump energy of 470 mJ/pulse. Data was acquired in a pump-probe delay range up to around 160 ps and with finer time steps between -2.5 to 6 ps. The Pd(111) reflex for this sample was observed on the 2D AGIPD detector, 3.5 m away from the sample. More than 100 000 measured 2D diffraction patterns were converted to the polar coordinates and the Bragg peaks were fitted with a Pseudo-Voigt function. Bragg peak parameters corresponding to the peak position, intensity and the peak's width in the radial and azimuthal directions were analyzed. The most pronounced signal was obtained from changes in the peak. We observed oscillations in the signal in the picosecond time range, together with an exponential decay time constant of $\tau \approx 110$ ps.

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Session Classification: Poster session with buffet

Track Classification: CDL2 (Photon Science)