

This DATSETNAME readme.txt file was generated on 2021/07/23. Updated 2022/06/02

GENERAL INFORMATION

Title of Dataset: 20210720_PtCeO2_TEM

Experiment name: Fluxional Behavior of Pt/CeO₂ at Room Temperature in Vacuum

Brief description of Dataset:

The dataset contains instances of transmission electron microscopy (TEM) *in-situ* movies of a heterogeneous catalyst consisting of 1 – 5 nm platinum (Pt) metal nanoparticles sitting on a cerium oxide (CeO₂) support. A total of 18,597 frames are used. The experimental data was recorded at room temperature at a base pressure of $\sim 10^{-6}$ Torr. The electron beam fluence during recording was $600\text{e}^-/\text{\AA}^2/\text{s}$. The instances are part of 25 videos, taken at a frame rate of 75 frames per second and each video may show up to 10 Pt nanoparticles in each frame. The instances show Pt particles in the size range 1 – 5 nm. In a subset of the frame series, the particles may become unstable and undergo structural dynamic re-arrangements. The periods of instability are punctuated by periods of relative stability. Consequently the nanoparticles show a variety of different sizes and shapes and are also viewed along many different crystallographic directions. Data was collected using a FEI Titan environmental transmission electron microscope operating at 287 kV. All images were acquired with a Gatan K3 camera direct electron camera operating in correlative double sampling (CDS) mode at full sensor resolution and at 75 frames-per-second exposure times. The movies are Gatan *in situ* dataset format and, on average, are 10 Gigabytes in size, consisting of 75 fps time-series of 3.4k x 3.4k images captured over 5–15 seconds (total of $\sim 375\text{--}1,125$ frames).

Images were acquired over a period of two days. The beam was blanked when images were not being acquired.

Unique sample ID:

17PtCeO₂ E2 from Joshua L. Vincent

Brief description of sample:

The sample consists of 17 wt.% Pt nanoparticles supported on CeO₂ nanocubes. The catalyst powder (taken from a vial with sample ID: E2) was dispersed on a clean Ta wire mesh with a dry-loading procedure. The catalyst-loaded mesh was placed in a Gatan Ta furnace hot stage and loaded into the microscope. A H₂ reduction (at about 0.4 Torr H₂ pressure) was performed for 2 hours at 400 °C prior to any imaging. The TEM sample is prepared as described here (J. L. Vincent and P. A. Crozier, Nature communications 2021 Vol. 12 Issue 1 Pages 1–13).

Date of data collection (single date, range, approximate date): 2021/07/20–21–22

Instrument used for data collection: FEI Titan ETEM in EFTEM mode, Gatan Tantalum hot stage, K3 camera in CDS mode

Funding sources or sponsorship that supported the collection of the data:

NSF CBET-1134464, (Josh)

NSF DMR-1840841 (Mai)

DOE, BES, DE-SC0004954 (Piyush)

DATA & FILE OVERVIEW

Brief description file list and directory structure:

The overall dataset consists of 25 *in situ* movies. Each *in situ* movie is stored in a parent folder having a specific name that follows a convention defined below. The naming convention provides context on the sample region, environmental condition, and time of capture, along with other relevant details, like the camera frame rate and electron dose rate, etc. The directory structure of the parent folder follows the Gatan

in situ dataset format. (Gatan Microscopy Suite (GMS) software version 3.43 or greater is required to open these K3 *in situ* datasets. Documentary videos showing how to work with the Gatan *in situ* data format are provided in the Gatan Media Library). In general, the directory of the *in situ* dataset is structured in accordance with the time sequence of data acquisition, i.e., “..\Hour_00\Minute_00\Second_00\..”, then “..\Hour_00\Minute_00\Second_01\..”, and so on. The seconds sub-folder, i.e., “..\Second_00\..”, contains a 1.0 second time-series file in Gatan .dm4 format. The name of this time-series file is prefixed with the same name as the parent folder and appended with a string to mark the time of acquisition, i.e., “_Hour_00_Minute_00_Second_00”. In this dataset, the 1.0 second time-series file is typically about 880 Megabytes in size and consists of 75 frames of 3.4k x 3.4k images. The individual K3 images are 8-bit unsigned integer data format.

Example dataset filename:

20210721JLV_PtCeO2_030103_Vacuum_600eA2s_75fps_1650kx_1854pm

Detailed description of folder/file naming convention:

The folder/file names are constructed from a number of short phrases, each separated by an underscore, i.e. ‘_’. In the example dataset file name above, the phrases and their meaning are as follows:

20210721JLV

Data acquired on 2021/07/21 by JLV.

PtCeO2

The catalyst sample consists of PtCeO₂ (specifically 17 wt.% Pt/CeO₂ catalyst labeled E2 by JLV).

File list (filenames, directory structure (for zipped files) and brief description of all data files):

OXOYOZ means:

“OX” Ceria Nanoparticle under observation

“OY” Condition of data capture (see below)

“OZ” Data captured at the same ceria nanoparticle but different locations.

For example: 010403 would mean “for condition 04, 1st ceria nanoparticle under observation, data collected at 3rd location on the same ceria nanoparticle”.

Magnification

1. 1.6MX (original pixel size = 0.01702nm, current pixel size = 0.00851nm)
2. 980KX (original pixel size = 0.02866nm, current pixel size = 0.013891nm)

Relationship between files, if important for context:

There might be images captured at same condition related to each other. For e.g., 010303 and 010305, would be images acquired of the same ceria nanoparticle region (i.e. #1) at the same environmental condition (i.e. #3) but at different times (i.e., #03 and #05).

METHODOLOGICAL INFORMATION

Description of methods used for collection/generation of data:

Aberration-corrected *in situ* HR-ETEM imaging of ceria-supported Pt nanoparticles under vacuum. Data captured under *in situ* conditions with the K3 camera (CDS mode, EFTEM mode, 75fps, full sensor resolution) at room temperature at the specific conditions listed below. The environmental TEM was operated at an accelerating voltage of 297 kV throughout the duration of the experiment. Images were acquired with the aberration corrector tuned to a negative C_s imaging (NCSI) mode. At the desired dose rate and a magnification of 980KX, the K3 sensor was registering approximately 51.5 e⁻/pixel/sec.

Experiment conditions:

condition 01: vacuum, 600e/A2/s

condition 05: vacuum, $P = 2.10 \cdot 10^{-6}$ torr, $600 \text{ e}/\text{Å}^2/\text{s}$
condition 06: vacuum, $P = 3.80 \cdot 10^{-7}$ torr, $600 \text{ e}/\text{Å}^2/\text{s}$
condition 11: vacuum, $P = 6.47 \cdot 10^{-7}$ torr, $600 \text{ e}/\text{Å}^2/\text{s}$

Software- or Instrument-specific information needed to open the data, including software and hardware version numbers: **Gatan Microscopy Suite (GMS) version 3.43 or higher is needed to open the *in situ* data.**

Standards and calibration information, if appropriate: **Pixel size was approximately calibrated on-the-fly during the experiment, but it may need further examination for a precise calibration.**

Describe any quality-assurance procedures performed on the data: **Image time-series were periodically opened during the experiment to inspect for artifacts or file corruption issues.**

SHARING/ACCESS INFORMATION

Licenses/restrictions placed on the data, or limitations of reuse: **none**

Recommended citation for the data: **Citation of authors, reference to "20210720-21-22 Fluxional PtCeO₂ 200C CO-O₂ K3 CDS" dataset.**