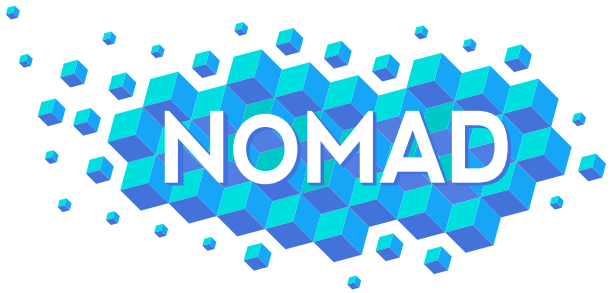
https://www.fairmat-nfdi.eu/fairmat/consortium



NOVEL MATERIALS DISCOVERY

https://nomad-lab.eu/

Ellipsometry Example and Tutorial in NOMAD

Activities Firefox Sep 21 16:31

NOMAD

localhost:3000/fairdi/nomad/latest/gui/about/information 130%

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About NOMAD

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NOMAD – Manage and Publish Materials Data

This is the *graphical user interface* (GUI) of NOMAD. It allows you to **search, access, and download all NOMAD data** in its *raw files* and *processed data* form. You can **upload and manage your own raw materials science data**. You can access all published data without an account. If you want to provide your own data, please login or register for an account.

You can learn more about NOMAD on its homepage, our documentation. There is also an FAQ and the more detailed uploader documentation.

Interactive Search

NOMAD extracts **rich metadata** from uploaded raw-data. Explore NOMAD's data by creating complex queries from interactive data visualizations of key properties, including the simulated composition/system, used method, upload metadata, as well as material classifications and available quantities. Or use the **Optimade** filter language to add arbitrarily nested queries.

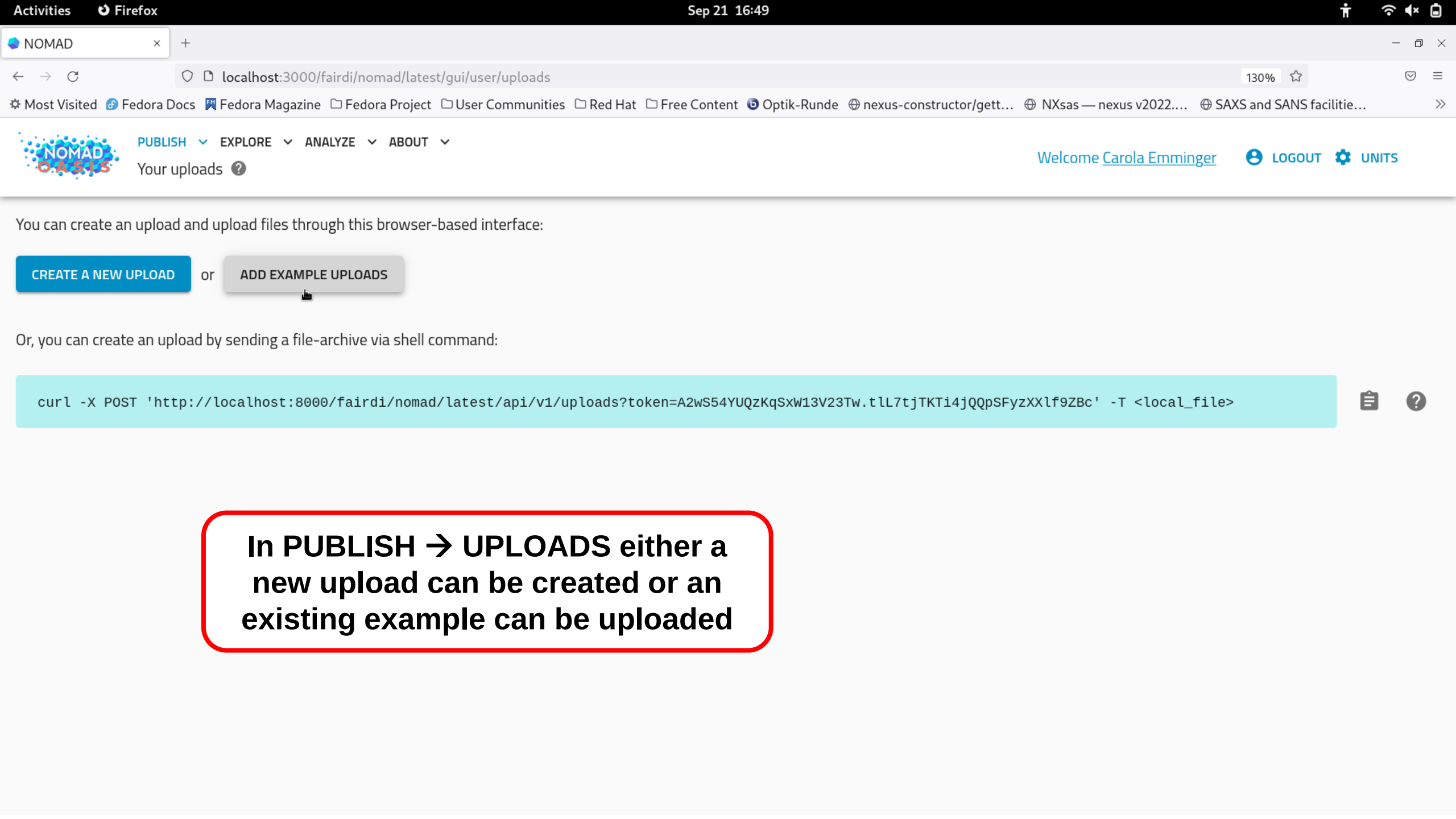
A common data format

NOMAD provides data in *processed* and *normalized* form in a machine processable and common hierarchical format. This *processed data*, i.e. the **NOMAD Archive**, is organized into nested sections of quantities with well defined units, data types, shapes, and descriptions. These definitions are called the **NOMAD Metainfo** and they can be browsed here.

What is shown on these slides is a developer's version of NOMAD, but the example will be integrated into NOMAD soon

NOMAD only uses cookies that are strictly necessary for this site's functionality

Read localhost


Activities
Firefox
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localhost:3000/fairdi/nomad/latest/gui/user/uploads
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ABOUT
Your uploads
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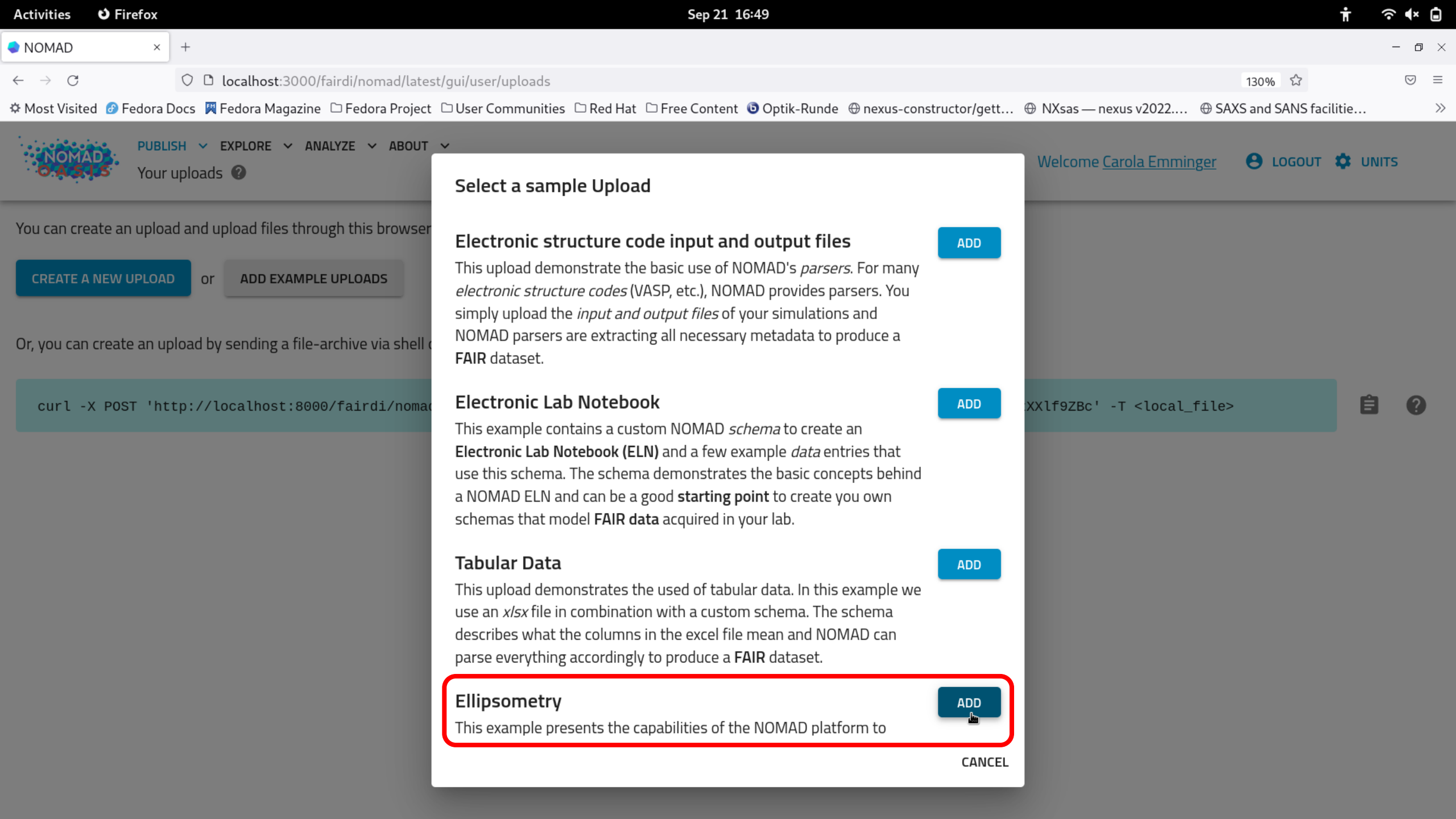
UNITS
You can create an upload and upload files through this browser-based interface:
CREATE A NEW UPLOAD
or
ADD EXAMPLE UPLOADS
Or, you can create an upload by sending a file-archive via shell command:
curl -X POST 'http://localhost:8000/fairdi/nomad/latest/api/v1/uploads?token=A2wS54YUQzKqSxW13V23Tw.tlL7tjTKTi4jQQpSFyzXXlf9ZBc' -T <local_file>
In PUBLISH → UPLOADS either a new upload can be created or an existing example can be uploaded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You can create an upload and upload files through this browser
CREATE A NEW UPLOAD
or
ADD EXAMPLE UPLOADS
Or, you can create an upload by sending a file-archive via shell
curl -X POST 'http://localhost:8000/fairdi/nomad
XXlf9ZBc' -T <local_file>
Select a sample Upload
Electronic structure code input and output files
ADD
This upload demonstrate the basic use of NOMAD's parsers. For many electronic structure codes (VASP, etc.), NOMAD provides parsers. You simply upload the input and output files of your simulations and NOMAD parsers are extracting all necessary metadata to produce a FAIR dataset.
Electronic Lab Notebook
ADD
This example contains a custom NOMAD schema to create an Electronic Lab Notebook (ELN) and a few example data entries that use this schema. The schema demonstrates the basic concepts behind a NOMAD ELN and can be a good starting point to create you own schemas that model FAIR data acquired in your lab.
Tabular Data
ADD
This upload demonstrates the used of tabular data. In this example we use an xlsx file in combination with a custom schema. The schema describes what the columns in the excel file mean and NOMAD can parse everything accordingly to produce a FAIR dataset.
Ellipsometry
ADD
This example presents the capabilities of the NOMAD platform to
CANCEL

Ellipsometry

upload id: oKItn96XQSieCGNTwkHn7Q

Each upload has its own upload id

README.md

Introduction

This example presents the capabilities of the NOMAD platform to store and standardize ellipsometry data. It shows the generation of a NeXus file according to the NXellipsometry application definition and a successive analysis of an example data set (measured values of the ellipsometric angles Psi and Delta of SiO2 on Si).

Viewing uploaded data

Below, you find an overview of your uploaded data. Click on the `> /` button to get a list of your data or select **FILES** from the top menu of this upload. You may add your own files to the upload or experiment with the pre-existing electronic lab notebook (ELN) example. The ELN follows the general structure of NOMAD ELN templates and you may refer to the documentation or a YouTube tutorial (~1h) for further information. When the ELN is saved a NeXus file will be generated from the provided example data. You may also view your supplied or generated NeXus files here with the H5Web viewer. To do so open the **FILES** tab and just select a `.nxs` file.

Activities Firefox Sep 21 17:05

NOMAD

localhost:3000/fairdi/nomad/latest/gui/user/uploads/upload/id/oKItn96XQSieCGNTwkHn7Q/entry/id/O3r5hUaa8xjPvPt8im_kJ3o2LsL_ 130%

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OVERVIEW FILES DATA LOGS

Metadata

type
Ellips
name
ellips.data.archive.json

comment
no comment
references
authors
Carola Emminger
datasets
no datasets

mainfile
ellips.data.archive.json
entry id
O3r5hUaa8xjPvPt8im_kJ3o2LsL_
material id
unavailable
upload id
oKItn96XQSieCGNTwkHn7Q

Ellips

Reader
ellips

Electronic Lab Notebook (ELN)

Nxdl
NXellipsometry.nxdl

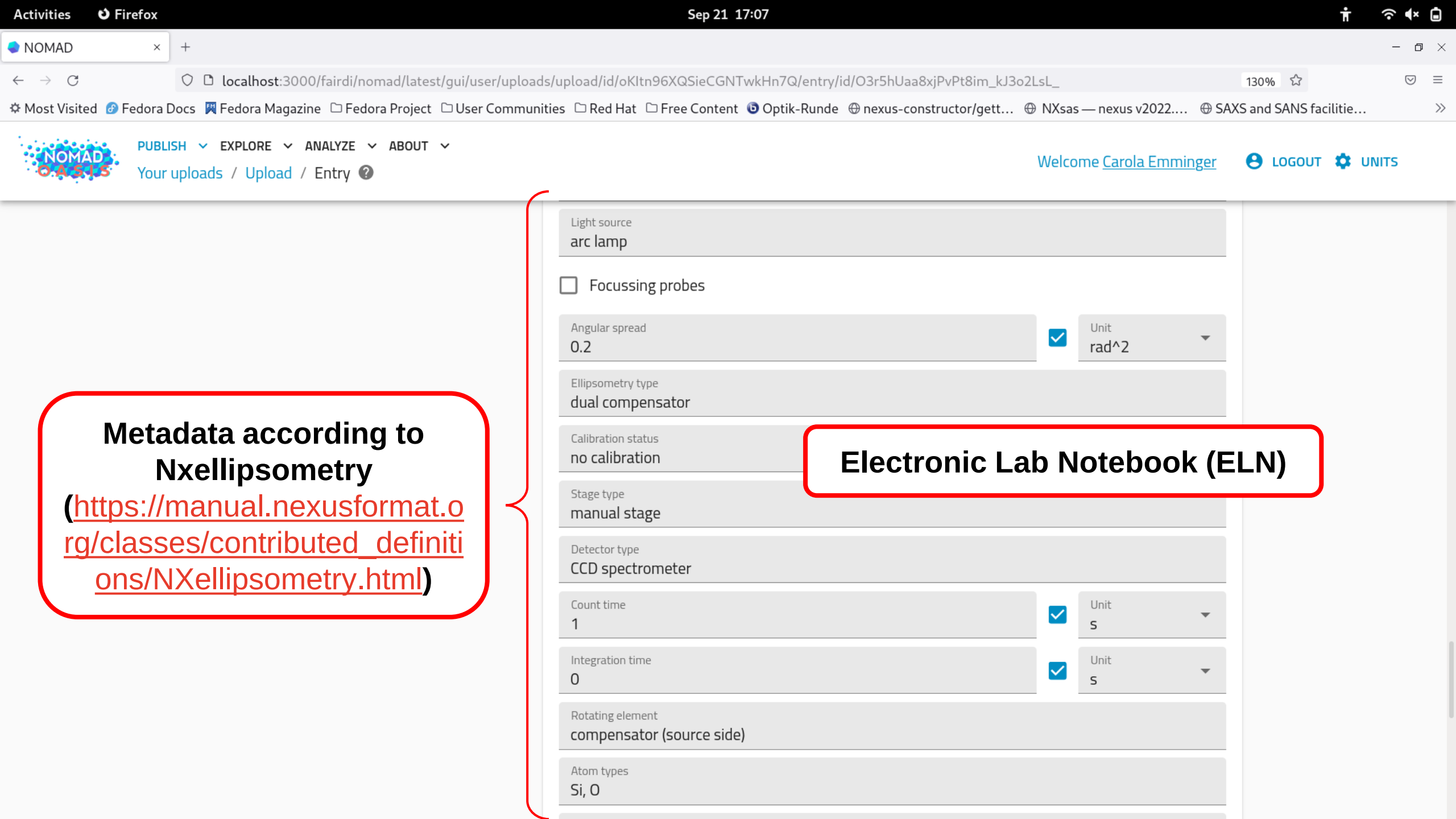
input_files
test-data.dat

input_files
eln_data.yaml

input_files

Output
SiO2onSi.ellips.nxs

Filename
test-data.dat


Activities
Firefox
Sep 21 17:07
NOMAD
localhost:3000/fairdi/nomad/latest/gui/user/uploads/upload/id/oKItn96XQSieCGNTwkHn7Q/entry/id/O3r5hUaa8xjPvPt8im_kJ3o2LsL_
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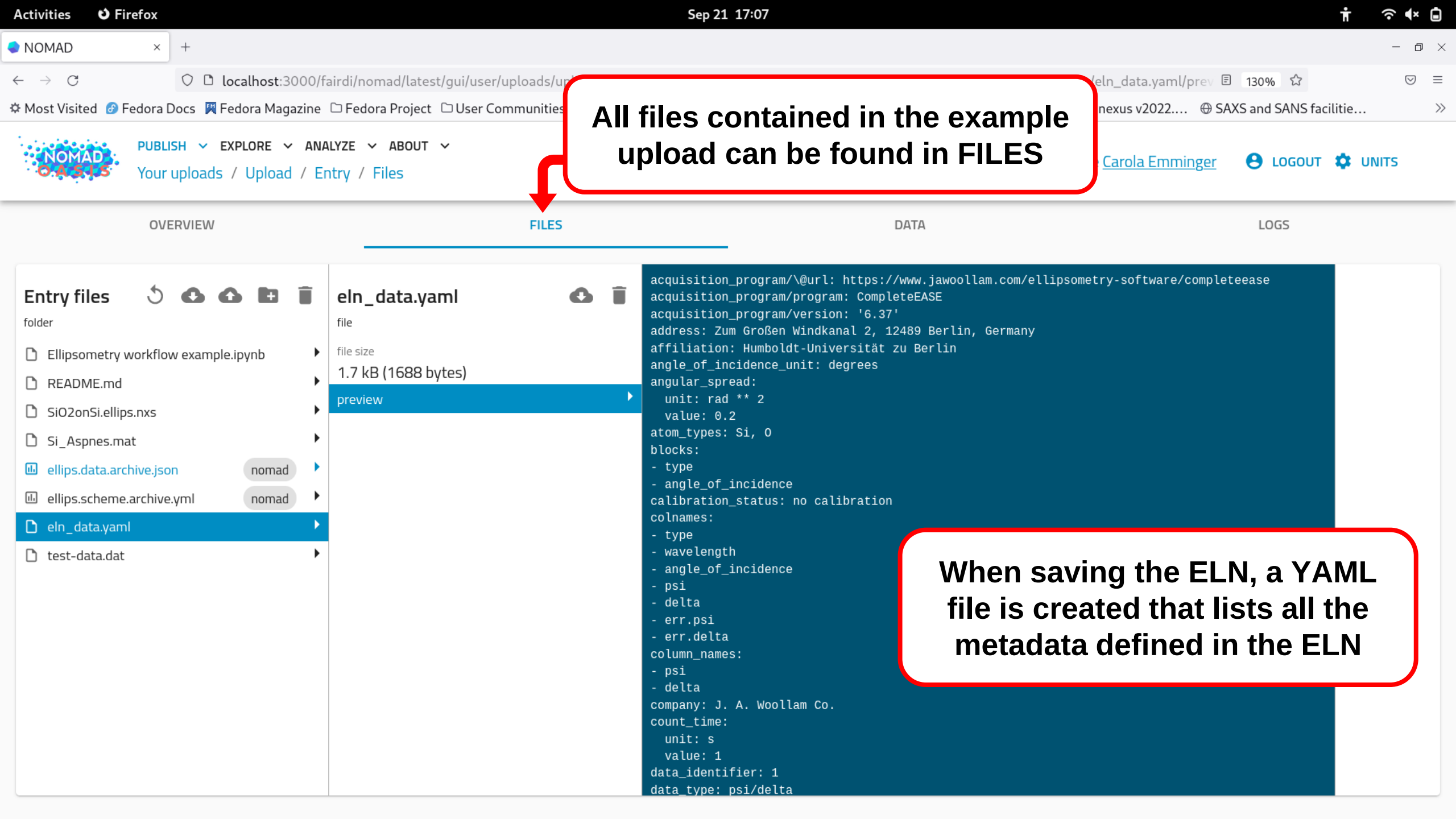
UNITS
Light source
arc lamp
Focussing probes
Angular spread
0.2
Unit
rad^2
Ellipsometry type
dual compensator
Calibration status
no calibration
Stage type
manual stage
Detector type
CCD spectrometer
Count time
1
Unit
s
Integration time
0
Unit
s
Rotating element
compensator (source side)
Atom types
Si, O
Metadata according to Nxellipsometry (https://manual.nexusformat.org/classes/contributed_definitions/NXellipsometry.html)
Electronic Lab Notebook (ELN)


Activities
Firefox
Sep 21 17:07
NOMAD
localhost:3000/fairdi/nomad/latest/gui/user/uploads/
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All files contained in the example upload can be found in FILES
OVERVIEW
FILES
DATA
LOGS
Entry files
folder
Ellipsometry workflow example.ipynb
README.md
SiO2onSi.ellips.nxs
Si_Aspnes.mat
ellips.data.archive.json
nomad
ellips.scheme.archive.yml
nomad
eln_data.yaml
test-data.dat
eln_data.yaml
file
file size
1.7 kB (1688 bytes)
preview
acquisition_program/\@url: https://www.jawoollam.com/ellipsometry-software/completeease
acquisition_program/program: CompleteEASE
acquisition_program/version: '6.37'
address: Zum Großen Windkanal 2, 12489 Berlin, Germany
affiliation: Humboldt-Universität zu Berlin
angle_of_incidence_unit: degrees
angular_spread:
unit: rad ** 2
value: 0.2
atom_types: Si, O
blocks:
- type
- angle_of_incidence
calibration_status: no calibration
colnames:
- type
- wavelength
- angle_of_incidence
- psi
- delta
- err.psi
- err.delta
column_names:
- psi
- delta
company: J. A. Woollam Co.
count_time:
unit: s
value: 1
data_identifier: 1
data_type: psi/delta
When saving the ELN, a YAML file is created that lists all the metadata defined in the ELN

Entry files

folder

- Ellipsometry workflow example.ipynb
- README.md
- SiO2onSi.ellips.nxs
- Si_Aspnes.mat
- ellips.data.archive.json nomad
- ellips.scheme.archive.yml nomad
- eln_data.yaml
- test-data.dat

test-data.dat

file

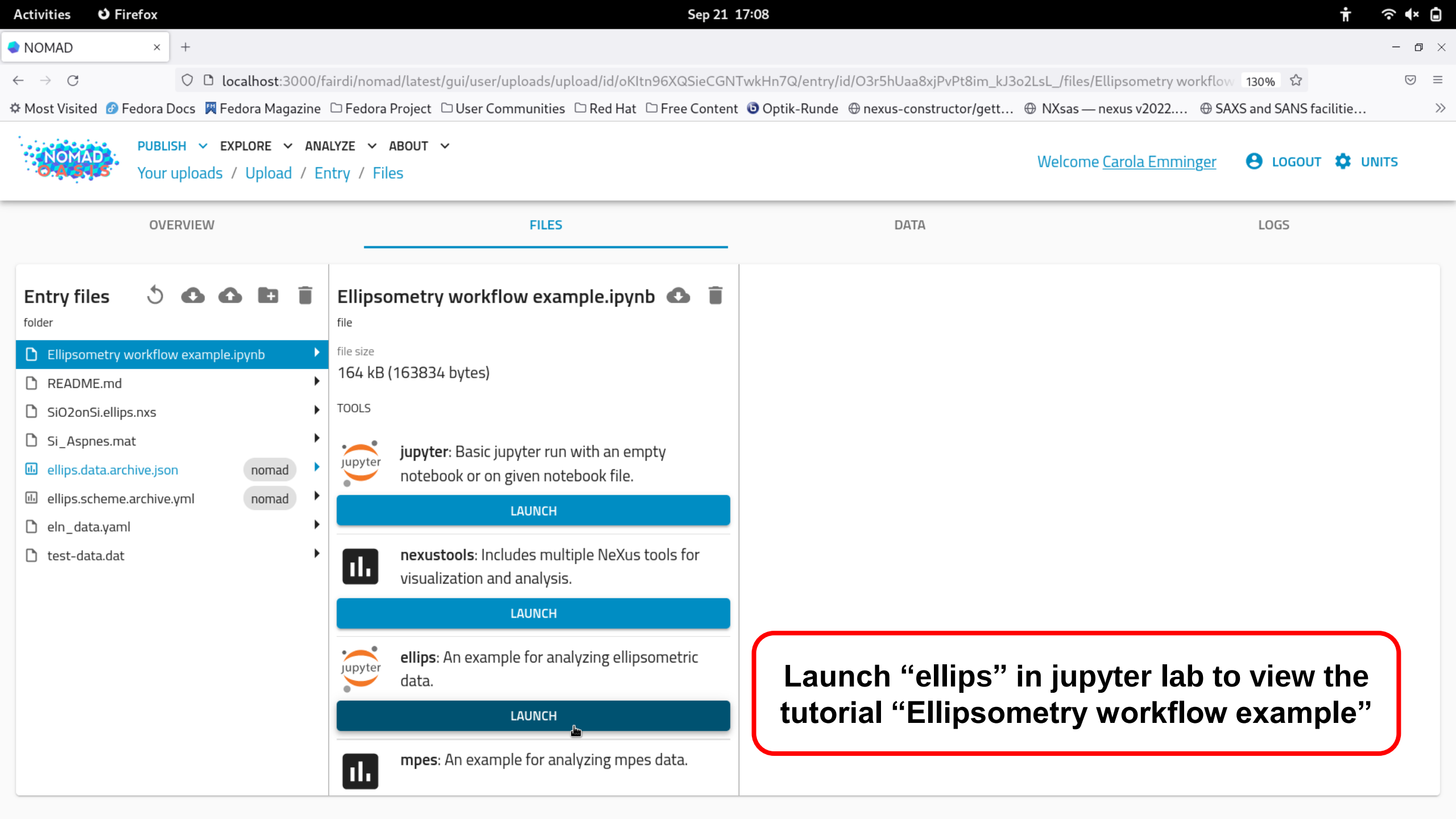
file size

482 kB (482497 bytes)

preview

The file containing the measured data

```
2nm SiO2 on Si on RC2
VASEmethod[EllipsometerType=4 , CompleteEASE=6.37, AcqTime=15.000, ZoneAve=1, Acq. Parameters=DE
Angstroms
E       1930.000000     50.000000       40.014217       142.127655      0.008585        0.034774
E       1940.000000     50.000000       40.026409       142.307449      0.007827        0.031627
E       1950.000000     50.000000       40.031204       142.483231      0.007221        0.029106
E       1960.000000     50.000000       40.045902       142.679901      0.006813        0.027399
E       1970.000000     50.000000       40.065468       142.866608      0.006478        0.025995
E       1980.000000     50.000000       40.077728       143.102463      0.006224        0.024925
E       1990.000000     50.000000       40.080673       143.409317      0.006016        0.024045
E       2000.000000     50.000000       40.082367       143.746017      0.005829        0.023258
E       2010.000000     50.000000       40.072388       143.990952      0.005649        0.022496
E       2020.000000     50.000000       40.073170       144.279099      0.005475        0.021767
E       2030.000000     50.000000       40.069405       144.611435      0.005311        0.021084
E       2040.000000     50.000000       40.066757       144.883820      0.005150        0.020417
E       2050.000000     50.000000       40.061028       145.150055      0.004993        0.019760
E       2060.000000     50.000000       40.055706       145.396118      0.004843        0.019128
E       2070.000000     50.000000       40.036533       145.661514      0.004703        0.018531
E       2080.000000     50.000000       40.017166       145.896454      0.004572        0.017967
E       2090.000000     50.000000       40.025864       146.114670      0.004443        0.017414
E       2100.000000     50.000000       40.028156       146.370560      0.004322        0.016892
E       2110.000000     50.000000       40.012478       146.607407      0.004227        0.016464
E       2120.000000     50.000000       40.007420       146.799438      0.004136        0.016055
E       2130.000000     50.000000       40.005928       147.055832      0.004045        0.015653
E       2140.000000     50.000000       40.001190       147.294281      0.003968        0.015308
E       2150.000000     50.000000       39.999153       147.531891      0.003896        0.014983
E       2160.000000     50.000000       39.998287       147.757156      0.003830        0.014690
E       2170.000000     50.000000       39.997860       147.958969      0.003769        0.014416
E       2180.000000     50.000000       40.001450       148.183533      0.003709        0.014154
E       2190.000000     50.000000       39.995445       148.426010      0.003648        0.013888
E       2200.000000     50.000000       39.998291       148.655228      0.003589        0.013635
```


Activities
Firefox
Sep 21 17:08
NOMAD
localhost:3000/fairdi/nomad/latest/gui/user/uploads/upload/id/oKItn96XQSieCGNTwkHn7Q/entry/id/O3r5hUaa8xjPvPt8im_kJ3o2LsL_/files/Ellipsometry workflow
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OVERVIEW
FILES
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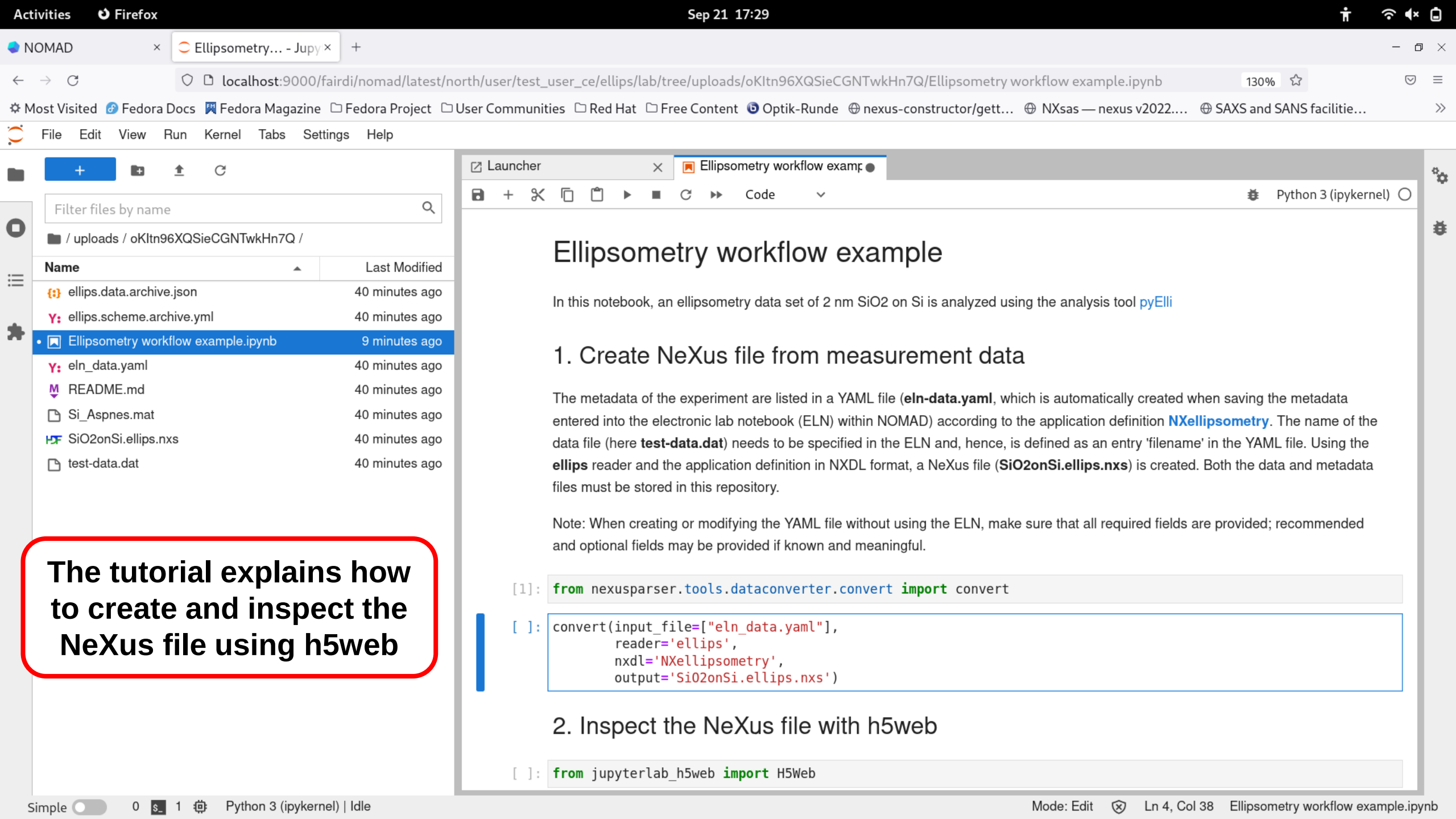
LOGS
Entry files
folder
Ellipsometry workflow example.ipynb
README.md
SiO2onSi.ellips.nxs
Si_Aspnes.mat
ellips.data.archive.json
nomad
ellips.scheme.archive.yml
nomad
eln_data.yaml
test-data.dat
Ellipsometry workflow example.ipynb
file
file size
164 kB (163834 bytes)
TOOLS
jupyter: Basic jupyter run with an empty notebook or on given notebook file.
LAUNCH
nexustools: Includes multiple NeXus tools for visualization and analysis.
LAUNCH
ellips: An example for analyzing ellipsometric data.
LAUNCH
mpes: An example for analyzing mpes data.
Launch “ellips” in jupyter lab to view the tutorial “Ellipsometry workflow example”


Activities
Firefox
Sep 21 17:29
NOMAD
Ellipsometry... - Jupy
localhost:9000/fairdi/nomad/latest/north/user/test_user_ce/ellips/lab/tree/uploads/oKltn96XQSieCGNTwkHn7Q/Ellipsometry workflow example.ipynb
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File
Edit
View
Run
Kernel
Tabs
Settings
Help
Filter files by name
/ uploads / oKltn96XQSieCGNTwkHn7Q /
Name
Last Modified
ellips.data.archive.json 40 minutes ago
ellips.scheme.archive.yml 40 minutes ago
Ellipsometry workflow example.ipynb 9 minutes ago
eln_data.yaml 40 minutes ago
README.md 40 minutes ago
Si_Aspnes.mat 40 minutes ago
SiO2onSi.ellips.nxs 40 minutes ago
test-data.dat 40 minutes ago
The tutorial explains how to create and inspect the NeXus file using h5web
Launcher
Ellipsometry workflow examp
Code
Python 3 (ipykernel)
Ellipsometry workflow example
In this notebook, an ellipsometry data set of 2 nm SiO2 on Si is analyzed using the analysis tool pyElli
1. Create NeXus file from measurement data
The metadata of the experiment are listed in a YAML file (eln-data.yaml, which is automatically created when saving the metadata entered into the electronic lab notebook (ELN) within NOMAD) according to the application definition NXellipsometry. The name of the data file (here test-data.dat) needs to be specified in the ELN and, hence, is defined as an entry 'filename' in the YAML file. Using the ellips reader and the application definition in NXDL format, a NeXus file (SiO2onSi.ellips.nxs) is created. Both the data and metadata files must be stored in this repository.
Note: When creating or modifying the YAML file without using the ELN, make sure that all required fields are provided; recommended and optional fields may be provided if known and meaningful.
[1]: from nexusparser.tools.dataconverter.convert import convert
[ ]: convert(input_file=["eln_data.yaml"],
reader='ellips',
nxdl='NXellipsometry',
output='SiO2onSi.ellips.nxs')
2. Inspect the NeXus file with h5web
[ ]: from jupyterlab_h5web import H5Web
Simple
0
1
Python 3 (ipykernel) | Idle
Mode: Edit
Ln 4, Col 38
Ellipsometry workflow example.ipynb

Activities Firefox Sep 21 17:30

NOMAD | Ellipsometry... - Jupy

localhost:9000/fairdi/nomad/latest/north/user/test_user_ce/ellips/lab/tree/uploads/oKItn96XQSieCGNTwkHn7Q/Ellipsometry workflow example.ipynb 130%

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File Edit View Run Kernel Tabs Settings Help

Filter files by name

/ uploads / oKItn96XQSieCGNTwkHn7Q /

Name	Last Modified
ellips.data.archive.json	41 minutes ago
ellips.scheme.archive.yml	41 minutes ago
Ellipsometry workflow example.ipynb	10 minutes ago
eln_data.yaml	41 minutes ago
README.md	41 minutes ago
Si_Aspnes.mat	41 minutes ago
SiO2onSi.ellips.nxs	seconds ago
test-[illegible].dat	41 minutes ago

Name: SiO2onSi.ellips.nxs
Size: 90.2 KB
Path: uploads/oKItn96XQSieCGNTwkHn7Q
Created: 2022-09-21 17:30:04
Modified: 2022-09-21 17:30:04
Writable: true

NeXus file: contains all the metadata and the measured data (+plots)

Launcher | Ellipsometry workflow examp

Markdown | Python 3 (ipykernel)

2. Inspect the NeXus file with h5web

[3]:
```
from jupyterlab_h5web import H5Web
```

[4]:
```
H5Web('SiO2onSi.ellips.nxs')
```

[4]:

SiO2onSi.ellips.nxs

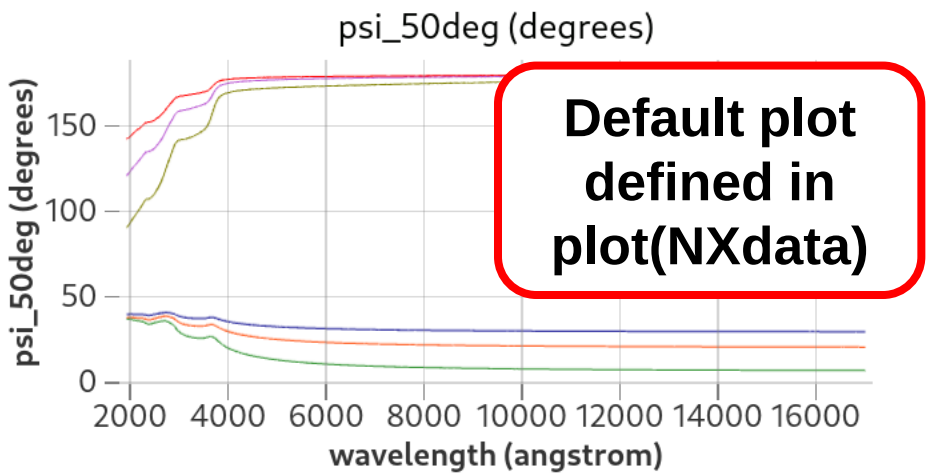
› entry NX

SiO2onSi.ellips.nxs | Display | Inspect | Feedback

NX Spectrum | X Linear | Y Linear | Auto-scale

n 1088

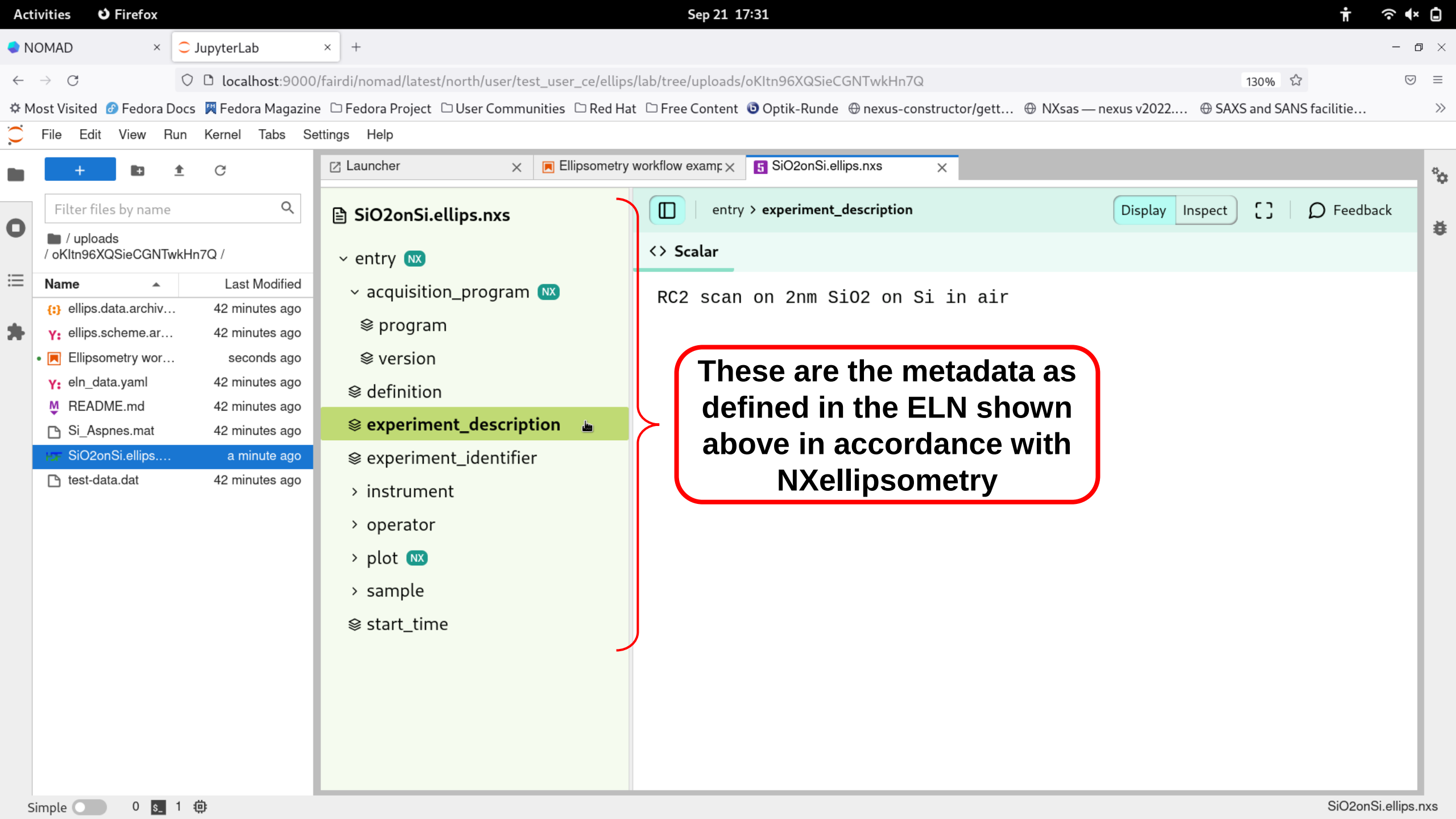
x D0



Default plot defined in plot(NXdata)

This is the end of the general template. Continue to fill the notebook based on **your own** post-processing of the *.nxs file.

Simple 0 1 Python 3 (ipykernel) | Idle Mode: Command Ln 1, Col 1 Ellipsometry workflow example.ipynb


Activities
Firefox
Sep 21 17:31
NOMAD
JupyterLab
localhost:9000/fairdi/nomad/latest/north/user/test_user_ce/ellips/lab/tree/uploads/oKItn96XQSieCGNTwkHn7Q
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Settings
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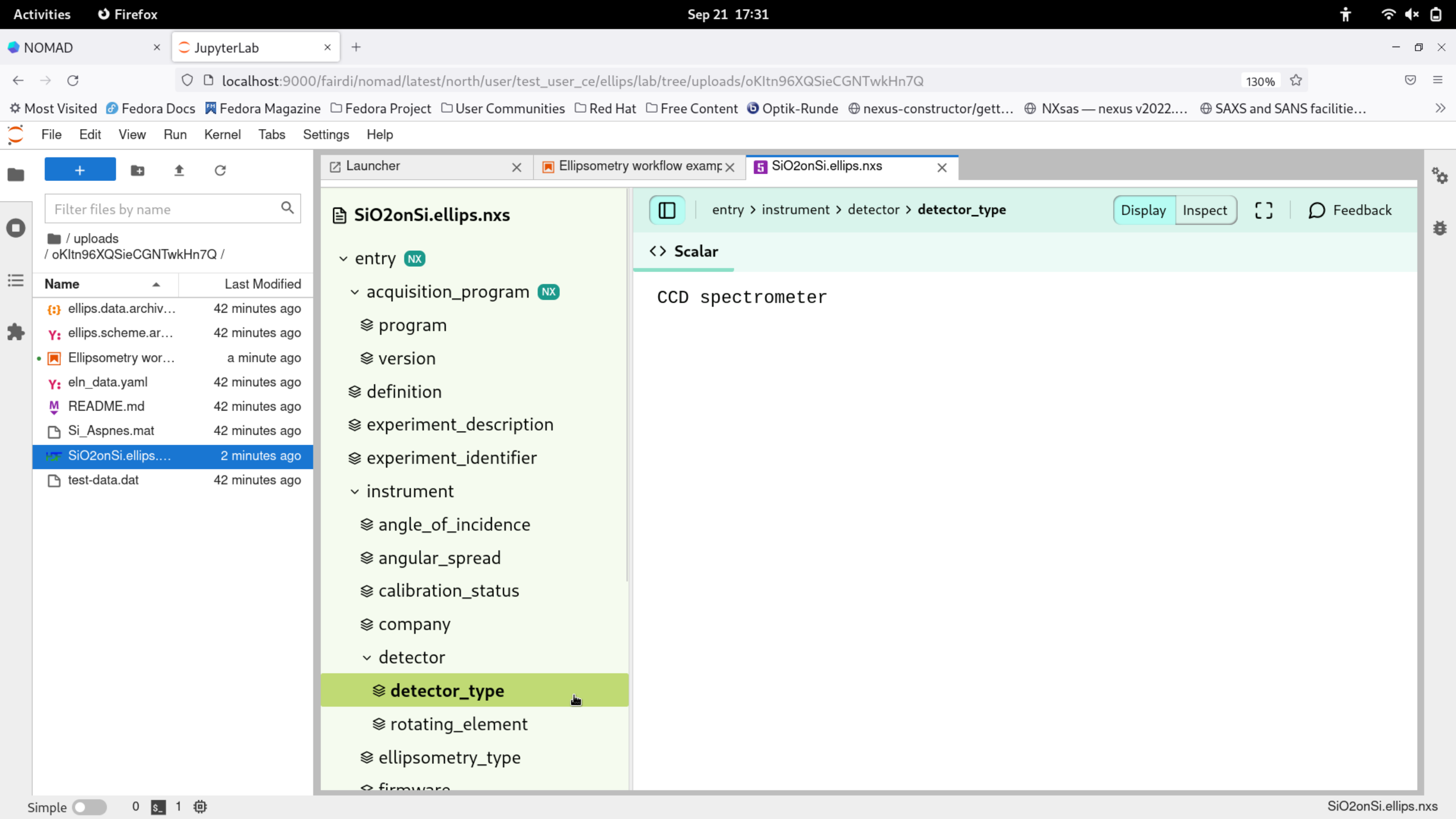
Launcher
Ellipsometry workflow examp
SiO2onSi.ellips.nxs
Filter files by name
/ uploads
/ oKItn96XQSieCGNTwkHn7Q /
Name
Last Modified
ellips.data.archiv... 42 minutes ago
ellips.scheme.ar... 42 minutes ago
Ellipsometry wor... seconds ago
eln_data.yaml 42 minutes ago
README.md 42 minutes ago
Si_Aspnes.mat 42 minutes ago
SiO2onSi.ellips.... a minute ago
test-data.dat 42 minutes ago
SiO2onSi.ellips.nxs
entry NX
acquisition_program NX
program
version
definition
experiment_description
experiment_identifier
instrument
operator
plot NX
sample
start_time
entry > experiment_description
Display
Inspect
Feedback
Scalar
RC2 scan on 2nm SiO2 on Si in air
These are the metadata as defined in the ELN shown above in accordance with NXellipsometry
Simple
0
1
SiO2onSi.ellips.nxs


Activities
Firefox
Sep 21 17:31
NOMAD
JupyterLab
localhost:9000/fairdi/nomad/latest/north/user/test_user_ce/ellips/lab/tree/uploads/oKItn96XQSieCGNTwkHn7Q
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Tabs
Settings
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Launcher
Ellipsometry workflow examp
SiO2onSi.ellips.nxs
Filter files by name
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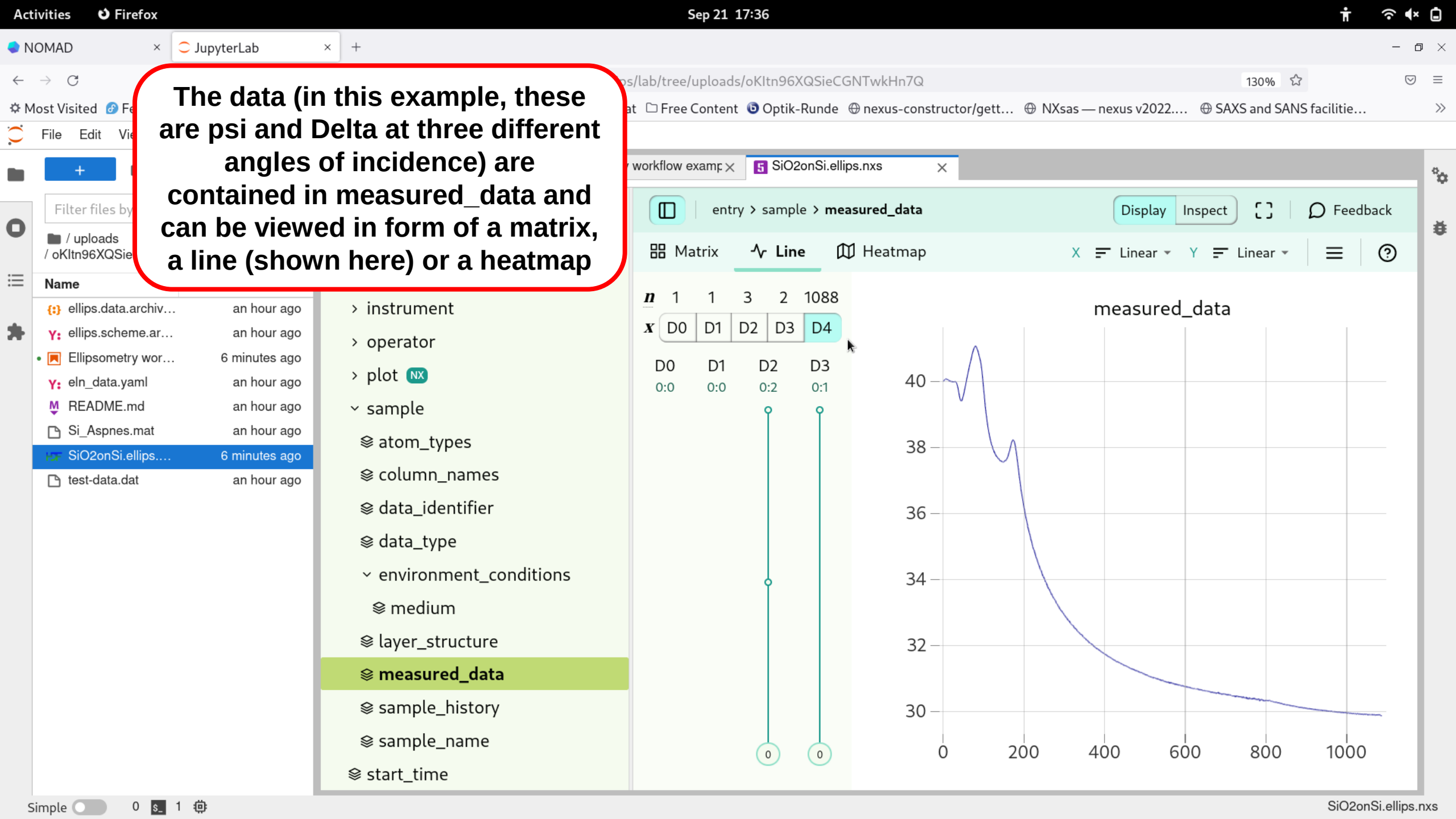
/ oKItn96XQSieCGNTwkHn7Q /
Name
Last Modified
ellips.data.archiv...
42 minutes ago
ellips.scheme.ar...
42 minutes ago
Ellipsometry wor...
a minute ago
eln_data.yaml
42 minutes ago
README.md
42 minutes ago
Si_Aspnes.mat
42 minutes ago
SiO2onSi.ellips....
2 minutes ago
test-data.dat
42 minutes ago
SiO2onSi.ellips.nxs
entry
NX
acquisition_program
NX
program
version
definition
experiment_description
experiment_identifier
instrument
angle_of_incidence
angular_spread
calibration_status
company
detector
detector_type
rotating_element
ellipsometry_type
entry > instrument > detector > detector_type
Display
Inspect
Feedback
Scalar
CCD spectrometer
Simple
0
1
SiO2onSi.ellips.nxs

The data (in this example, these are psi and Delta at three different angles of incidence) are contained in measured_data and can be viewed in form of a matrix, a line (shown here) or a heatmap



Questions or Comments?

If you have questions or comments regarding the example, please feel free to contact us:

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