



# NeXus Application Definition Developments at FAIRmat

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## FAIRmat @ NFDI

- NFDI – German National Research Data Infrastructure  
9 projects started in 2020  
10 projects starts in 2021

...

- **FAIRmat project**  
5 years  
9 institutes  
52 research groups  
14 M€





# FAIR Data Infrastructure for Condensed-Matter Physics and the Chemical Physics of Solids

## 7 project Area

- A – Synthesis
- B – Experiments
- C – Theory and Computation
- D – Digital Infrastructure
- E – Use-case Demonstrators
- F – User Support, Training, and Outreach
- G – Administration and Coordination

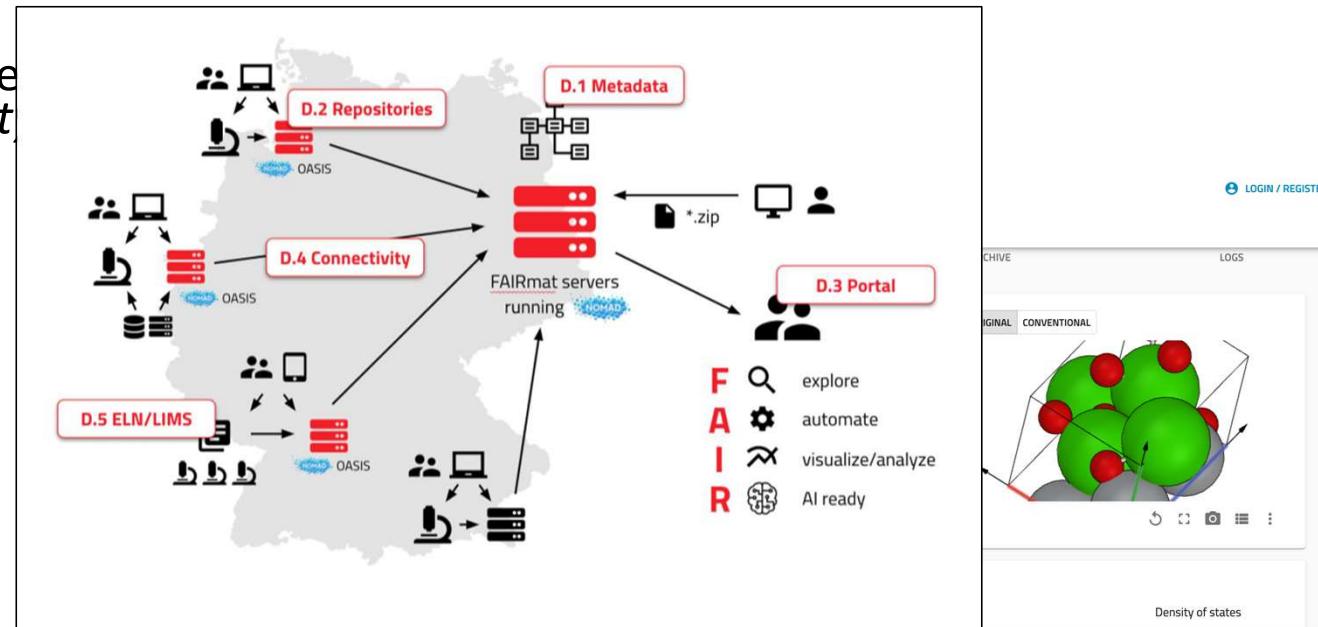




# Novel Materials Discovery



- Biggest database in Materials Science  
*more than 100 million high-quality entries*
- Encyclopedia
- Artificial Intelligence Toolkit
- Data Center @ MPCDF
- Local OASIS deployments
- Modern Technology
  - Backend with **Python Flask** and Fastapi, MongoDB, Elasticsearch
  - Workflows with Celery, RabbitMQ
  - Frontend with **Javascript**: React, MaterialUI
  - Docker, Kubernetes,
  - AAI using Keycloak





# Novel Materials Discovery



- **NOMAD HUB (*NOMAD Data Center at HU Berlin*)**
  - connecting Synthesis – Experiments – Calculations
  - Integrate experimental data (e.g. NeXus)
  - NeXus Application Definitions for
    - *Electron Microscopy*
    - *Angle Resolved Photoemission*
    - *Core-level Spectroscopy*
    - *Optical Spectroscopy*
    - *Atom-probe Tomography*

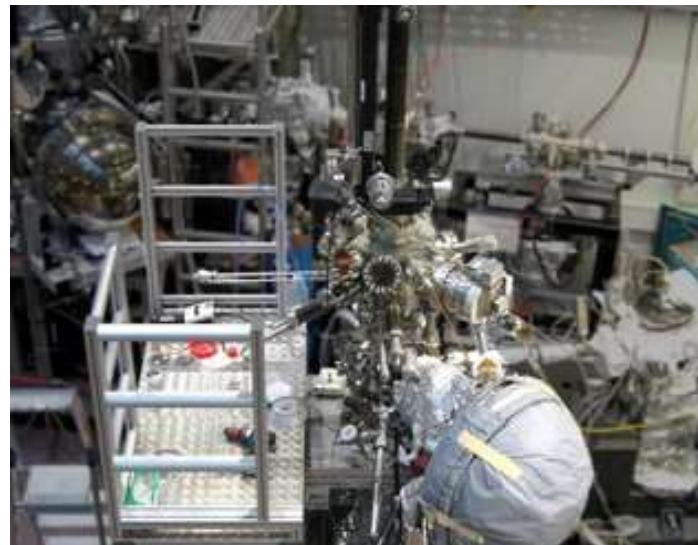


# NeXus Application Definitions



- **Experiment**

- *Instrumentation*
- *Sample* Preparation
- Sample Environment
- Monitors and Detectors
- Data Processing



- **Synthesis**

- *Sample* History
- *Processes*
- *Characterisation*
- *Notes*





# NeXus Application Definitions

## • Experiment

- *Instrumentation*
- *Sample Preparation*
- *Sample Environment*
- *Motors and Detectors*
- *Data Processing*

## • Synthesis

- *Sample History*
- *Processes*
- *Characterisation*
- *Notes*

## NeXus:

- Hierarchical Data Modelling

- Definitions (*glossary/ontology*)

- Automated documentation

- Extendable (*NXDL*)

- Community STANDARD

- NXDL <-> NXS (*hdf5*)

## Verification and Validation

- Data Visualisation

## Processes:

- Spin coating

- PVD deposition

- Solution preparation

- Hotplate annealing

- ...

## Measurements:

- XRD

- XRF measurement

- Hyperspectral PL imaging

- Raman spectroscopy

- J-V measurement

- ...

## Samples

## Processing Setup:

- PVD chamber

- Hot plate

- Spin coater

- ...

## Characterisation Setup:

- XRD PANalyticalMPD for thin films

- XRF Mapper M4 Tornado

- ...

## Targets for PLD and sputtering

## Chemicals

## Setup status:

- crucible filling tracking

- ...





# NeXus Applications

- Bag of Words (YAML)

SingleWordName:  
EnglishExpression:  
Definition:  
QuantityType:  
Unit:  
Shape:  
Axes:  
Relationships:



SingleWordName	English Expression	Definition	Quantity Type	Unit	Shape	Axes	Relationships
SpectrumEnergy	Photon energy	Wavelength at which the spectrum was measured	Array(float)	eV	N		
AngleOfIncidence	Angle of Incidence	Angle of incidence at which the spectrum was measured	float	degree		1	
DataMM	Mueller Matrix	Mueller Matrix Spectrum for a given energy spectrum and angle of incidence	Matrix(Float)		N,16		
Dataalso	Standard Ellipsometry Data	standard ellipsometry spectrum for a given energy spectrum and angle of incidence	Matrix(Float)		N,2		
DataJones	Jones matrix	Jones matrices for a given energy spectrum and angle of incidence	Matrix(ComplexFloat)		N,4		
DataDepolarisation	Depolarisation	Depolarisation of the spectrum	Array(float)		N		
DataJQI	Jones Quality Index	Jones quality index (measure of the depolarization factor of the Sample)					
LayerStructure	Layer structure of the Sample	Description of the layer structure	String				
SampleDescription	Sample description	Description of the Sample, e.g., structural properties of the involved materials	string				
Mode	Measurement Mode	Reflection or transmission mode					
Temperature	Temperature	Temperature at which the Spectrum was taken	float	K		1	
Time	Time	Time step	float	s			
InitSystem	Initial coordinate System	Definition of the initial coordinate System	string				
EulerAngles	Euler angles	Euler angles in the zxz notation describing the sample orientation	Array(float)			3	
Date	Date and time	date and time when the spectrum was measured	date				
IntegrationTime	Integration Time	Accumulation time for the spectrum	float	s		1	
RevolutionPol	Revolution Polarizer	Number of revolutions of the Polarizer	int			1	
RevolutionAna	Revolution Analyzer	Number of revolutions of the Analyzer	int			1	
PositionPol	Position polarisator	Positions of the Polarizer	Array(float)		N		
PositionAna	Position analyzer	Positions of the Analyzer	Array(float)		N		
RevolutionCompS	Revolution Compensator	Number of revolutions of the Compensator at the source side	int			1	
RevolutionCompD	Revolution Compensator	Number of revolutions of the Compensator at the detector side	int			1	
PositionCompS	Position Compensators	Position of the Compensator at the source side	Array(float)		N		
PositionCompD	Position Compensators	Position of the Compensator at the detector side	Array(float)		N		
EllipsometerType	Ellipsometer Type	Type of the Ellipsometer (e.g. RCE, PME)	string				
EllipsometerConfigurat	Configuration	Configuration of the Ellipsometer (e.g. PCSA)	string				
EllipsometerManufacut	Manufacturer	manufacturer of the ellipsometer	string				
EllipsometerModel	Model	Model of the Ellipsometer	string				
Comments	Comments		string				
WindowCorrection	Window Correction	Correction of window effects	Array(float)		N		



# NeXus Application Definitions

- Bag of Words (YAML)
- Hierarchical and modular structure (YAML)  
(with references to the Bag of Words)

SingleWordName:  
EnglishExpression:  
Definition:  
QuantityType:  
Unit:  
Shape:  
Axes:  
Relationships:

instrument:  
model:  
company:  
construction year:  
hardware version:  
software version:  
bandwidth:  
light source:  
focussing probes:  
data\_correction:  
description: specify of the recorded data are co  
angular spread:  
description: specify the angular spread caused by  
type: numeric  
unit: radian  
ellipsometry type:  
- rotating analyzer  
- rotating analyzer with analyzer compensator  
- rotating analyzer with polarizer compensator





# NeXus Applications

- Bag of Words (YAML)
- Hierarchical and modular structure (YAML)  
(with references to the Bag of Words)
- Use of already existing NeXus definitions (YAML)

SingleWordName:  
EnglishExpression:  
Definition:  
QuantityType:  
Unit:  
Shape:  
Axes:  
Relationships:

- (NXentry):
  - exists: required
  - doc: to be defined
  - experiment\_identifier:
    - exists: required
    - doc: Unique identifier of the experiment
    - experiment\_description:
      - exists: required
      - start\_time(NX\_DATE\_TIME):
        - exists: required
        - unit: NX\_TIME
      - program\_name:
        - doc: Commercial or otherwise distributed
      - program\_version:
        - doc: Either version with build number or specific of the recorded data are considered
      - instrument(NXinstrument):
        - doc: General properties of the instrument
        - exists: required
      - model:
        - rotating analyzer:
          - doc: The name of the instrument
        - rotating an... # if the nx\_class or type is nx\_char
        - rotating an... # if the exists argument is optional
      - company:



# NeXus Applications

- Bag of Words (YAML)
- Hierarchical and modular structure (YAML) (with references to the Bag of Words)
- Use of already existing NeXus definitions
- New NeXus App Definitions (NXDL)  
<https://fairmat-experimental.github.io/nexus-fairmat-proposal/>

SingleWord:  
EnglishExpression:  
Definition:  
QuantityType:  
Unit:  
Shape:  
Axes:  
Relationship:

A screenshot of a web-based application definition page. At the top is a red header with a white snowflake icon and the text "NeXus-FAIRmat". Below the header is a dark teal sidebar containing navigation links such as "FAIRmat-NeXus Proposal", "NeXus Documentation", "Navigation", and "Quick search". The main content area has a white background and contains several sections: "Status" (application definition, extends NXobject), "Description" (Draft application definition for ellipsometry measurements, including complex systems up to variable angle spectroscopic ellipsometry. In this application definition, times should be specified always together with a UTC offset.), "Symbols" (Variables used throughout the document, e.g. dimensions and important parameters), "Groups cited" (NX\_TIME, NXaperture, NXcollection, NXdata, NXdetector, NXentry, NXinstrument, NXsample, NXsubentry, NXtransformations, NXuser), and "Structure". The "Structure" section includes definitions for "ENTRY" (required NXentry), "definition" (required NX\_CHAR), "An application definition for ellipsometry. Such experiments may be as simple as identifying how a reflected beam of light with a single wavelength changes its polarization state, to a variable angle spectroscopic ellipsometry experiment. The application definition defines: - elements of the experimental instrument - calibration information if available - parameters used to tune the state of the sample - sample description"), "Obligatory value: NXellipsometry", "@version" (required NX\_CHAR), and "@url" (required NX\_CHAR).

## NXellipsometry

### Status:

application definition, extends NXobject

### Description:

Draft application definition for ellipsometry measurements, including complex systems up to variable angle spectroscopic ellipsometry. In this application definition, times should be specified always together with a UTC offset.

### Symbols:

Variables used throughout the document, e.g. dimensions and important parameters

**N\_wavelength:** Size of the energy / wavelength vector used

**N\_variables:** How many variables are saved in a measurement (e.g. Psi and Delta, Mueller matrix).

**N\_angles:** Number of incident angles used

**N\_p1:** Number of sample parameters scanned

**N\_time:** Number of time points measured

### Groups cited:

NX\_TIME, NXaperture, NXcollection, NXdata, NXdetector, NXentry, NXinstrument, NXsample, NXsubentry, NXtransformations, NXuser

### Structure:

**ENTRY:** (required) NXentry

"This is the application definition describing ellipsometry experiments. Such experiments may be as simple as identifying how a reflected beam of light with a single wavelength changes its polarization state, to a variable angle spectroscopic ellipsometry experiment. The application definition defines: - elements of the experimental instrument - calibration information if available - parameters used to tune the state of the sample - sample description"

**definition:** (required) NX\_CHAR

An application definition for ellipsometry.

Obligatory value: NXellipsometry

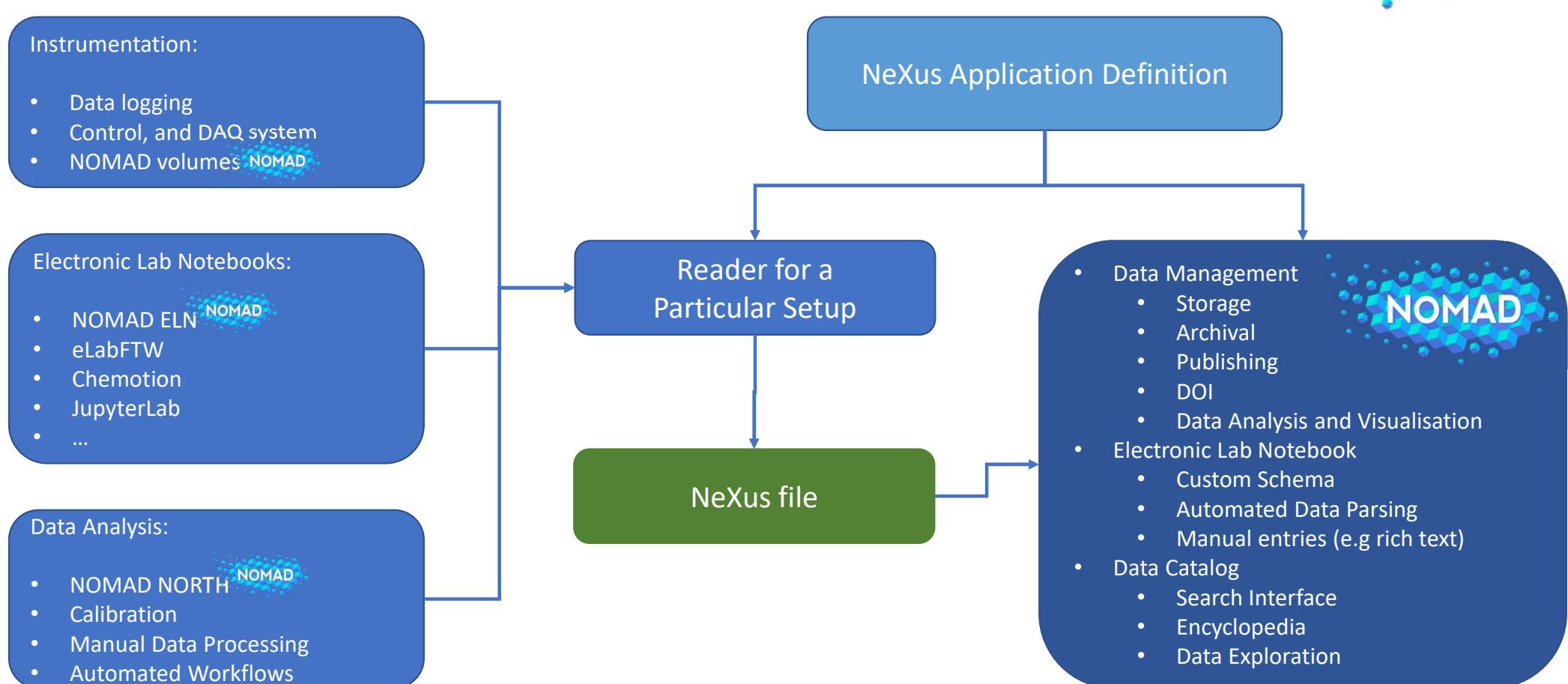
**@version:** (required) NX\_CHAR

Version number to identify which definition of this application definition was used for this entry/data.

**@url:** (required) NX\_CHAR



# Data & App Def in Use





# NeXus in NOMAD

NOMAD Metainfo Browser

PUBLISH EXPLORE ANALYZE ABOUT

source nomad

search

- nxus** (sub section definition)
  - SUB SECTION DEFINITIONS
  - nx\_application\_apm**
  - nx\_application\_archive**
  - nx\_application\_arxes**
  - nx\_application\_cansAS**
  - nx\_application\_directtof**
  - nx\_application\_tofraw**
  - nx\_application\_ellipsometry**
  - nx\_application\_TIME**
  - nx\_application\_nion**
  - nx\_application\_fluo**
  - nx\_application\_indirecttof**
  - nx\_application\_iproc**
  - nx\_application\_lauetof**
  - nx\_application\_monopd**
  - nx\_application\_mpes**
  - nx\_application\_electronanalyser**
  - nx\_application\_energydispersion**
  - nx\_application\_calibration**
  - nx\_application\_mx**
  - nx\_application\_refscan**
  - nx\_application\_reftof**
  - nx\_application\_sas**
  - nx\_application\_sastof**
  - nx\_application\_scan**
  - nx\_application\_spe**
  - nx\_application\_sqm**
  - nx\_application\_stxm**
  - nx\_application\_tas**
  - nx\_application\_tofnpd**
  - nx\_application\_tofsingle**
  - nx\_application\_tomo**
  - nx\_application\_tomophase**
  - nx\_application\_tomoproc**
- nx\_application\_ellipsometry** (sub section definition)
  - DESCRIPTION
  - This is the application definition for ellipsometry measurements, including complex systems up to variable angle spectroscopic ellipsometry. In this application definition, times should be specified always together with a UTC offset.
  - LINKS
  - nexus manual**
  - PROPERTIES
  - nx\_kind: group**
  - nx\_optional: false**
  - BASE SECTION
  - NXobject
  - SUB SECTION DEFINITIONS
  - nx\_group\_ENTRY (repeats)**
  - USAGE
  - SHOW USAGE**
- nx\_group\_ENTRY** (sub section definition)
  - DESCRIPTION
  - An application definition for ellipsometry.
  - LINKS
  - nexus manual**
  - PROPERTIES
  - nx\_kind: field**
  - nx\_type: NX\_CHAR**
  - nx\_optional: false**
  - BASE SECTION
  - definitionField
  - SUB SECTION DEFINITIONS
  - nx\_attribute\_version**
  - USAGE
  - SHOW USAGE**
- nx\_field\_definition** (sub section definition)
  - DESCRIPTION
  - An application definition for ellipsometry.
  - LINKS
  - nexus manual**
  - PROPERTIES
  - nx\_kind: attribute**
  - nx\_optional: false**
  - BASE SECTION
  - versionAttribute
  - SUB SECTION DEFINITIONS
  - nx\_value**
  - nx\_name**
  - QUANTITY DEFINITIONS
  - nx\_name**
  - nx\_value**
  - USAGE
  - SHOW USAGE**
- nx\_attribute\_version** (sub section definition)
  - DESCRIPTION
  - Version number to identify which definition of this application definition was used for this entry/data.
  - LINKS
  - nexus manual**
  - PROPERTIES
  - nx\_kind: attribute**
  - nx\_optional: false**
  - BASE SECTION
  - versionAttribute
  - SUB SECTION DEFINITIONS
  - nx\_value**
  - nx\_name**
  - QUANTITY DEFINITIONS
  - nx\_name**
  - nx\_value**
  - USAGE
  - SHOW USAGE**



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### Groups cited:

[NX\\_TIME](#), [NXaperture](#), [NXcollection](#), [NXdata](#), [NXdetector](#), [NXentry](#), [NXinspector](#), [NXsample](#), [NXsubentry](#), [NXtransformations](#), [NXuser](#)

### Structure:

#### ENTRY: (required) [NXentry](#)

"This is the application definition describing ellipsometry experiments. Such experiments may be as simple as identifying how a reflected beam of light with a single wavelength changes its polarization state, to a variable angle spectroscopic ellipsometry experiment. The application definition defines: - elements of the experimental instrument - calibration information if available - parameters used to tune the state of the sample - sample description"

#### definition: (required) [NX\\_CHAR](#)

An application definition for ellipsometry.

Obligatory value: [NXellipsometry](#)

#### @version: (required) [NX\\_CHAR](#)

Version number to identify which definition of this application definition was used for this entry/data.

#### @url: (required) [NX\\_CHAR](#)

URL where to find further material (documentation, examples) for this application definition

Watch

### Navigation

- FAIRmat-NeXus Proposal
- NeXus Documentation
  - [NeXus: User Manual](#)
  - [Examples of writing and reading](#)
  - [NeXus data files](#)
  - [NeXus: Reference Documentation](#)
  - [NeXus Community](#)
  - [Installation](#)
  - [NeXus Utilities](#)
  - [About these docs](#)
- MPES Structure
- Ellipsometry Structure
- Electron Microscopy Structure
- Atom Probe Microscopy Structure

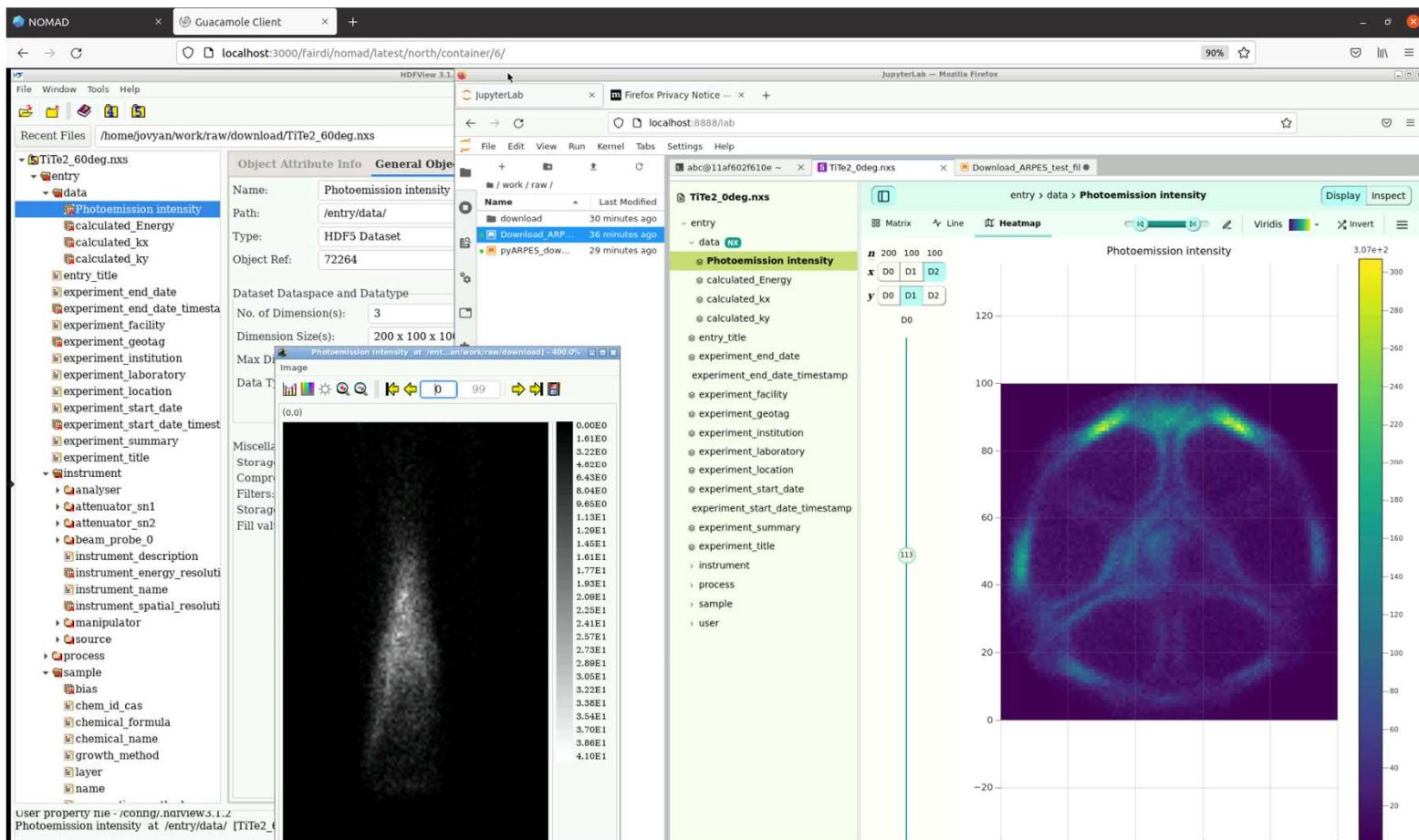
Quick search

Google search

global Nexus manual Go



# NOMAD Remote Tools Hub





# NOMAD ELN



PUBLISH EXPLORE ANALYZE ABOUT

Your uploads / Upload / Entry / Data

Welcome Jose Marquez LOGOUT UNITS

OVERVIEW FILES DATA LOGS

search

Entry section

SUB SECTIONS

results metadata

**data**

Sample section

QUANTITIES

Sample owner: Pepe Marquez

Sample id: 1988

Sample name: ELN sample

Creation datetime: 16/03/2022 18:44

Institute: HU Berlin

Description

0 WORDS POWERED BY TINY

Processes section

SUB SECTIONS

**pvd\_evaporation**

- pvd\_deposition
- ebeam\_evaporation
- hotplate\_annealing
- tubefurnace\_annealing
- rtp\_annealing
- spin\_coating
- chemical\_bath\_deposition

PVDEvaporation section

QUANTITIES

Operator: Pepe Marquez

Datetime: 02/03/2022 18:45

Instrument: PVD-P

Chemicals

Creates layer

Comments

0 WORDS POWERED BY TINY

substrate\_temperature quantity

PLOT

Substrate\_temperature (K)

process\_time (s)

VALUE

305.5632  
305.5641  
305.5660  
305.5679  
305.5681  
305.5690  
305.5699  
305.5712  
305.5765  
305.5778  
305.5795  
305.5854  
In\_values  
K

Number crucibles

data\_file: PVD\_Process\_data.csv

process\_time = 9647 vector

set\_substrate\_temperature = 9647 vector

substrate\_temperature = 9647 vector

chamber\_pressure = 9647 vector



# NOMAD with H5Web



NOMAD with H5Web interface showing a 2D diffraction pattern.

The interface includes:

- OVERVIEW**: Shows a list of entry files, including "mpes.test - Copy.hdf5".
- FILES**: Displays the contents of "mpes.test - Copy.hdf5", specifically an "NX Image" dataset.
- DATA**: A 2D plot showing the data (counts) as a function of  $k_x$  (1/ $\text{\AA}$ ) and  $k_y$  (1/ $\text{\AA}$ ). The plot shows a bright central spot with a surrounding diffuse halo.
- TOOLS**: Includes "hyperspy: Run hyperspy on an arbitrary .hdf5 file." and "H5Web".
- PREVIEW**: Shows a preview of the "H5Web" tool.

Plot details:

- Dimensions**:  $n = 100 \times 100 \times 100 \times 50$
- Coordinates**:  $x = [D0 | D1 | D2 | D3]$ ,  $y = [D0 | D1 | D2 | D3]$
- Labels**:  $D2$ ,  $0.99$ ,  $D3$ ,  $0.49$
- Axes**:  $k_x$  (1/ $\text{\AA}$ ) from -2.5 to 1.5,  $k_y$  (1/ $\text{\AA}$ ) from -1.4 to 1.4
- Color Scale**: Blues color bar ranging from 0 to 2000000 (200060192 bytes).
- Tools**: Includes "Invert", "Linear", "Flip Y", and "Keep ratio".