UNIVERSITÄT
LEIPZIG

FAIRmat

FAIRmat for Ellipsometry

Why to store and exchange ellipsometry and related data?

- Supporting material for papers (figures are limited in papers)
- Available for :
  - Further analysis / experiment
  - Comparison with other samples
- …

Dipole analysis of the dielectric function of color dispersive materials: Application to monoclinic Ga_2O_3

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(Received 2 February 2016; revised manuscript received 27 May 2016; published 22 July 2016)

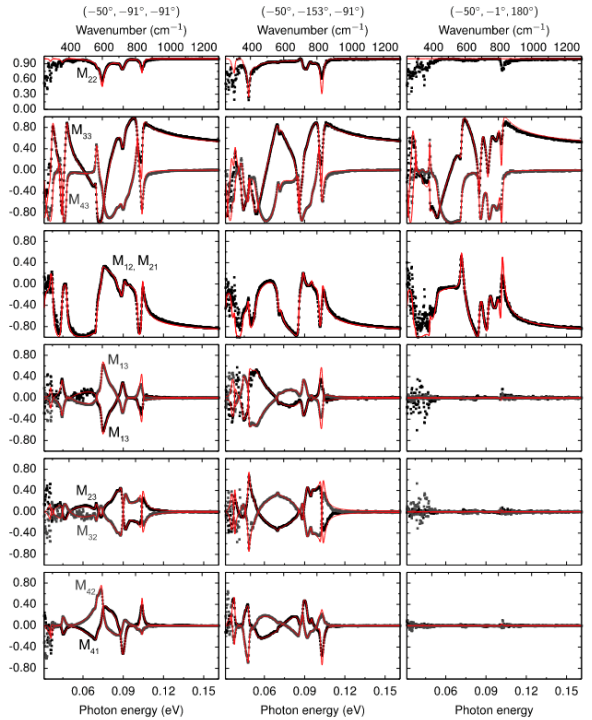
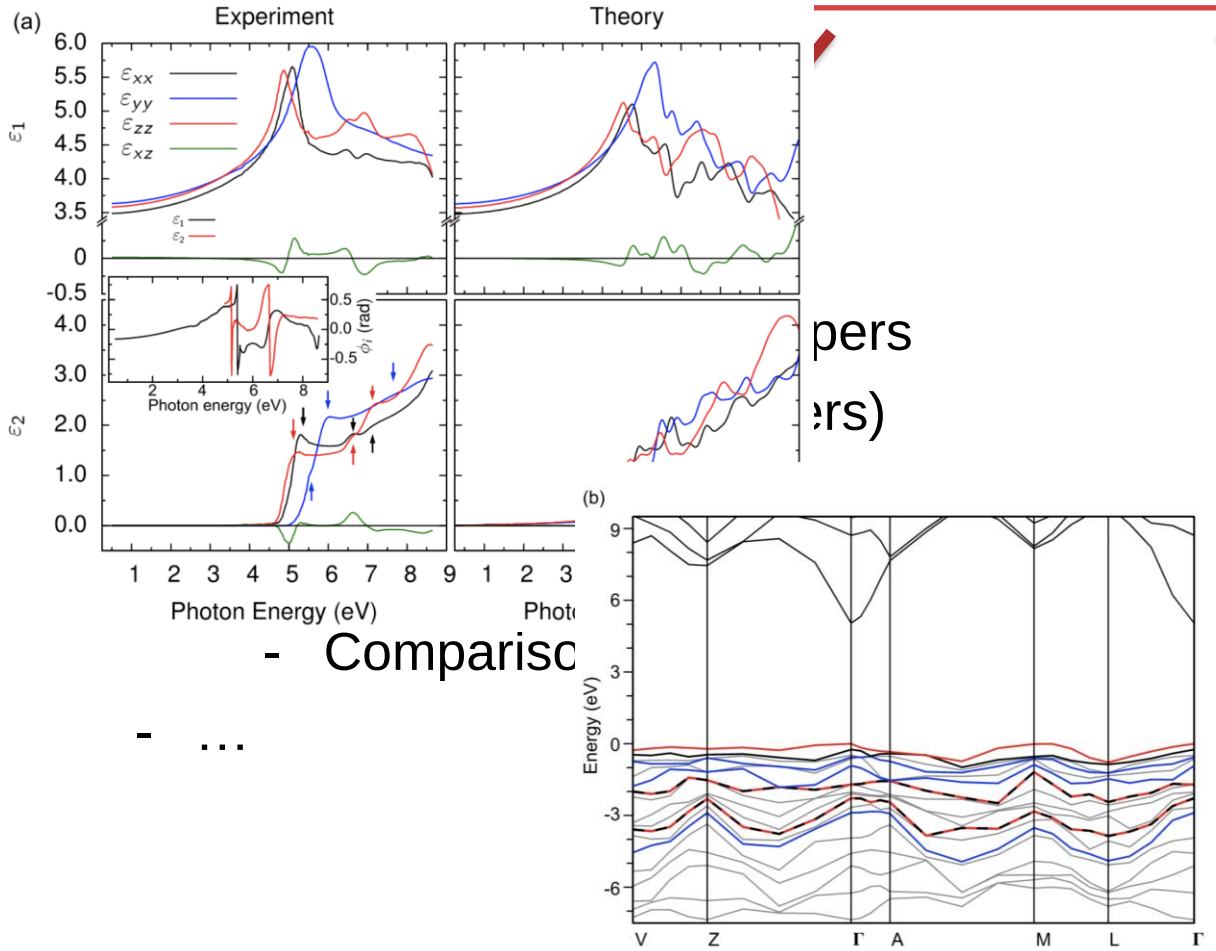


FIG. 3. Experimental (symbols) and calculated (lines) infrared spectra of the MM elements of a β-Ga_2O_3 bulk single crystal for an angle of incidence of 70°. The corresponding orientation of the crystal is given by the Euler angles on top of each column in the *yzx* notation.

Why to store and exchange ellipsometry and related data?



- Comparisc
- …

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ers)

- Analysis of the data of different setups and experiments for deeper understanding

- Verification of the results
- Test of theory
- …

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- Supporting material for papers (figures are limited in papers)
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- …

Within own and external groups

Storage of ellipsometry data

- Technology partners (e.g.):

SEMILAB

ACCURION
solutions for science

HORIBA

SENTECH

Problem:

- Each technology partner has its own file format
- Within a technology partner the file format can be different

Ellipsometry data

- **Ellipsometry data depends on:**
  - Sample properties (orientation, layer structure, …)
  - Angle of incidence
  - Experimental setup (PSA, PSC, PSMA, …)
  - Detection mode (integration time, polarizer setting, …)
  - Excitation condition (time resolution, …)
  - Environment (temperature, stress and strain, gas, ...)
  - …

- **What we want:**
  - Store meta information of the experimental conditions. / environment
  - Exchange data within the group and with colleagues

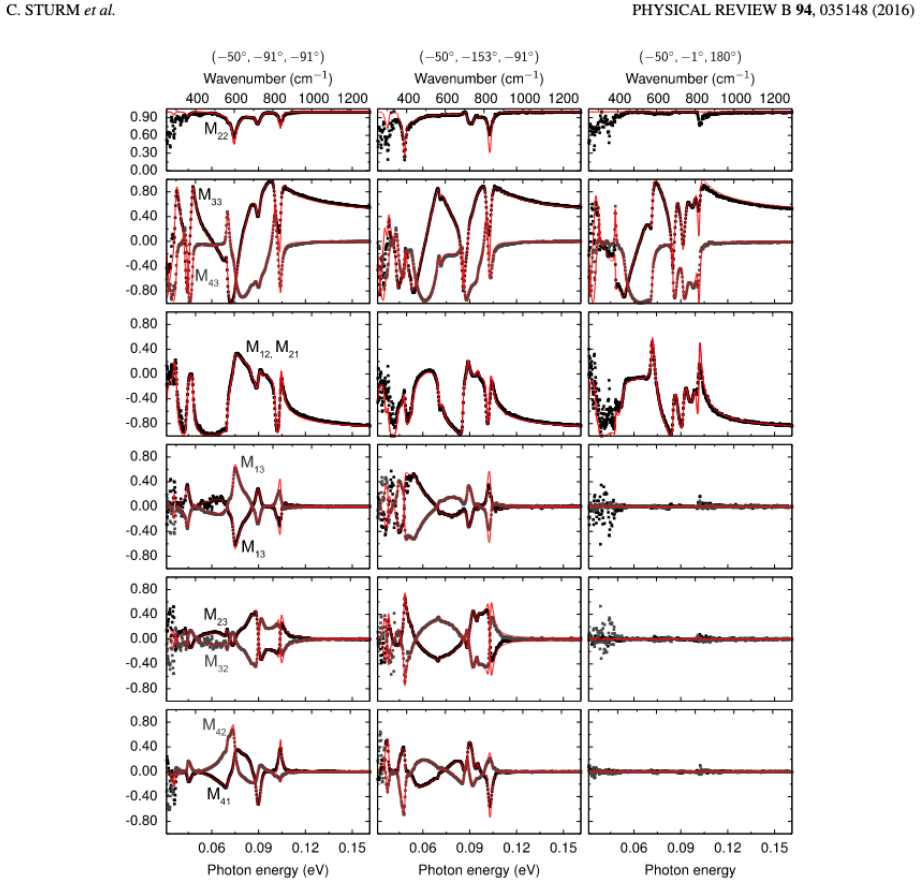

FIG. 3. Experimental (symbols) and calculated (lines) infrared spectra of the MM elements of a β-Ga_2O_3 bulk single crystal for an angle of incidence of 70°. The corresponding orientation of the crystal is given by the Euler angles on top of each column in the yzx notation.

How to exchange and store experimental data
and the corresponding meta information

- **Make data F**indable, **A**ccessible, **I**nteroperable, and **R**epurposable
- **Define (NeXus) Application definition**

FAIRmat

APPLICATION DEFINITION

User Manual and Reference Documentation

fairmat-experimental.github.io/nexus-fairmat-proposal

NeXus-FAIRmat

Proposal of NeXus expansion for FAIRmat data.

Watch

Navigation

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Welcome to the user manual of th

https://www.nexusformat.org/

NeXus

NeXus is developed as an international standard by scientists and programmers representing major scientific facilities in Europe, Asia, Australia, and North America in order to facilitate greater cooperation in the analysis and visualization of neutron, x-ray, and muon data.

Ellipsometry Structure

Introduction

Ellipsometry is an optical characterization method to describe optical properties of interfaces and thickness of films. The measurements are based on determining how the polarization state of light changes upon transmission and reflection. Interpretation is based on Fresnel equations and numerical models of the optical properties of the materials.

In the application definition we provide a minimum set of description elements allowing for a reproducible recording of ellipsometry measurements.

New Application Definitions

We created one application definition:

NXellipsometry:
A general application definition for ellipsometry measurements, including complex systems up to variable angle spectroscopic ellipsometry.

Base Classes Extended in Application Definitions

We use existent base classes in application definitions and add descriptors:

NXinstrument
Added fields to add information that is important for an ellipsometry setup, such as the ellipsometer type, the light source, the type of the sample stage, or the angle(s) of incidence, as well as information on calibration, focussing probes, data correction etc.

NXdetector
Added fields to describe spectroscopic detection with polarization (e.g. rotating analyzer).

3.3.3.17. NXellipsometry

NXellipsometry was accepted by NeXus as a contributed definition

https://manual.nexusformat.org/classes/contributed_definitions/NXellipsometry.html

Status:

application definition, extends NXobject

Description:

Ellipsometry, complex systems, up to variable angle spectroscopy.

Information on ellipsometry is provided, e.g. in:

- H. Fujiwara, Spectroscopic ellipsometry: principles and applications, John Wiley & Sons, 2007.
- R. M. A. Azzam and N. M. Bashara, Ellipsometry and Polarized Light, North-Holland Publishing Company, 1977.
- H. G. Tompkins and E. A. Irene, Handbook of Ellipsometry, William Andrew, 2005.

Open access sources:

- https://www.angstromadvanced.com/resource.asp
- https://pypolar.readthedocs.io/en/latest/

Review articles:

- T. E. Jenkins, "Multiple-angle-of-incidence ellipsometry", J. Phys. D: Appl. Phys. 32, R45 (1999), https://doi.org/10.1088/0022-3727/32/9/201
- D. E. Aspnes, "Spectroscopic ellipsometry - Past, present, and future", Thin Solid Films 571, 334-344 (2014), https://doi.org/10.1016/j.tsf.2014.03.056
- R. M. A. Azzam, "Mueller-matrix ellipsometry: a review", Proc. SPIE 3121, Polarization: Measurement, Analysis, and Remote Sensing, (3 October 1997), https://doi.org/10.1117/12.283870
- E. A. Irene, "Applications of spectroscopic ellipsometry to microelectronics", Thin Solid Films 233, 96-111

ELLIPSOMETRY STRUCTURE

- Metadata are defined in the Application Definition **NXellipsometry**
- Metadata include information about:
  - The operator (name, affiliation etc.)
  - the ellipsometer (type, light source, detector etc.)
  - the sample and its environment
  - …
- Entries can be required, recommended, and optional.

B4: Optical spectroscopy

Introduction

Ellipsometry is an optical characterization method to describe optical properties of interfaces and thickness of films. The measurements are based on determining how the polarization state of light changes upon transmission and reflection. Interpretation is based on Fresnel equations and numerical models of the optical properties of the materials.

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NXdetector
Added fields to describe spectroscopic detection with polarization (e.g. rotating analyzer).

NXaperture
Added fields to define parameters that describe windows (e.g. windows of a UHV cryostat), such as the thickness and the orientation angle of the window, as well as reference data to calculate window effects.

https://fairmat-experimental.github.io/nexus-fairmat-proposal

General Structure

- General metadata, such as experiment identifier, user(s), start time etc.
- INSTRUMENT:
  - Ellipsometer (model, company, firmware etc.)
  - Light source
  - Stage
  - Detector
  - …
- SAMPLE:
  - Sample name, history, data identifier etc.
  - Data type (e.g. psi and Delta, Mueller matrix, etc.)
  - Measured data
  - Environment conditions
- Derived parameters (e.g. depolarization)
- plot(NXdata): default view of data

→ Details will be discussed on Friday

General Structure

- General metadata, such as experiment ic
- INSTRUMENT:
  - Ellipsometer (model, company, firmware etc.)
  - Light source
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  - Detector
  - …
- SAMPLE:
  - Sample name, history, (
  - Data type (e.g. psi and I
  - Measured data
  - Environment condition
- Derived parameters (e.g. depolarization)
- plot(NXdata): default view of data

→ YAML:

```
62   (NXellipsometry):
63     (NXentry):
64   >   doc: |…
77
78   >   definition:…
87
88   >   experiment_identifier:…
94
95   >   experiment_description:…
       start_time(NX_DATE_TIME):…
       acquisition_program(NXprocess):…
       (NXuser):…
       (NXinstrument):…
532  >   (NXsample):…
718
719  >   derived_parameters(NXprocess):…
726
727  >   plot(NXdata):…
```

NeXus Definition Language (NXDL) Data Types
https://manual.nexusformat.org/nxdl-types.html

NeXus base classes
https://manual.nexusformat.org/classes/base_classes/index.html#base-class-definitions

NXellipsometry

https://fairmat-experimental.github.io/nexus-fairmat-proposal/1c3806dba40111f36a16d0205cc39a5b7d52ca2e/classes/contributed_definitions/NXellipsometry.html#nxellipsometry

Status:

applicatic

Description:

Ellipsome

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- D. E. 571.

be created ideally in a deterministic manner.

operator: (required) NXuser

Contact information of at least the user of the instrum performed this experiment. Adding multiple users if re

name: (required) NX_CHAR

Name of the user.

affiliation: (required) NX_CHAR

Name of the affiliation of the user at the point in tir was performed.

address: (required) NX_CHAR

Full address (street, street number, ZIP, city, count

email: (required) NX_CHAR

Email address of the user.

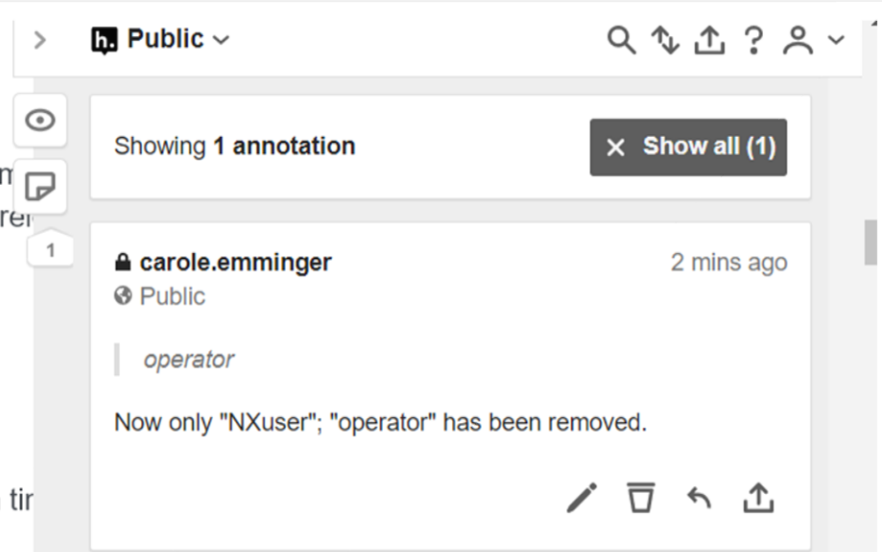
orcid: (recommended) NX_CHAR

Author ID defined by https://orcid.org/.

telephone_number: (recommended) NX_CHAR

Official telephone number of the user.

INSTRUMENT: (required) NXinstrument



Please feel free to leave comments, questions or suggestions

NeXus-FAIRmat

Proposal of NeXus expansion for FAIRmat data.

Watch

Navigation

FAIRmat-NeXus Proposal

NeXus Documentation

- NeXus: User Manual
- Examples of writing and reading NeXus data files
- NeXus: Reference Documentation
- NeXus Community

Ellipsometry Application Definition

→ YAML file can be read by any editor

! NXellipsometry.yaml ×

optical_spectroscopy > ! NXellipsometry.yaml > { } (NXellipsometry)

```
 8
 9   category: application
10 > doc: | ···
45
46 > symbols: ···
61
62   (NXellipsometry):
63     (NXentry):
64 >     doc: | ···
77
78 >     definition: ···
87
88 >     experiment_identifier: ···
94
95 >     experiment_description: ···
99
100 >    start_time(NX_DATE_TIME): ···
102
103 >    acquisition_program(NXprocess): ···
119
120 >    (NXuser): ···
141
142 >    (NXinstrument): ···
531
532 >    (NXsample): ···
718
719 >    derived_parameters(NXprocess): ···
726
727 >    plot(NXdata): ···
736
```

```
46   symbols:
47     doc: "Variables used throughout the document, e.g. dimensions and important parameters"
48     N_wavelength: "Size of the energy or wavelength vector used, the length of
49       NXinstrument/spectrometer/wavelength array"
50     N_variables: "How many variables are saved in a measurement. e.g. 2 for Psi
51       and Delta, 16 for Mueller matrix elements, 15 for normalized
52       Mueller matrix, 3 for NCS, the length of NXsample/column_names"
53     N_angles: "Number of incident angles used, the length of
54       NXinstrument/angle_of_incidence array"
55
56     N_p1:
57       "Number of sample parameters scanned, if you varied any of the parameters
58       such as temperature, pressure, or pH, the maximal length of the arrays
59       specified by NXsample/environment_conditions/SENSOR/value if it exists."
60     N_time: "Number of time points measured, the length of NXsample/time_points"
```

The Symbols table describes keywords used in this NXDL file to designate array dimensions.

ellipsometer type, light source, sample stage, angle(s) of incidence, information on calibration, focusing probes, data correction etc.

sample and material properties, the sample environment (e.g. refractive index of surrounding medium), experimental conditions (e.g. temperature, pressure, pH value etc.).

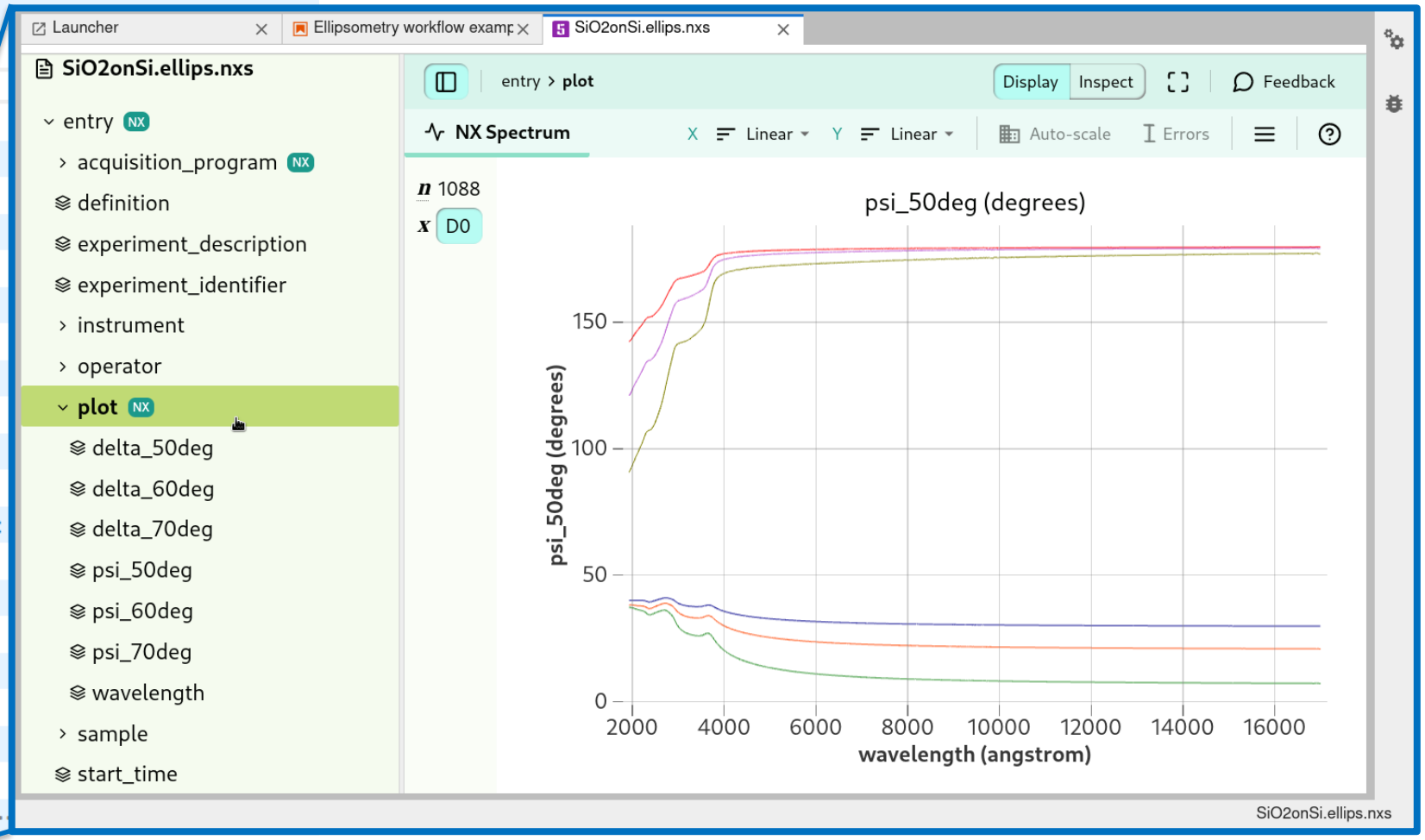
Ellipsometry Application Definition

NXellipsometry.yaml

optical_spectroscopy > NXellipsometry.yaml > { } (NXellipsometry)

```
  category: application
  doc: |
  symbols:
  (NXellipsometry):
    (NXentry):
      doc: |
      definition:
      experiment_identifier:
      experiment_description:
      start_time(NX_DATE_TIME):
      acquisition_program(NXprocess):
      (NXuser):
      (NXinstrument):
      (NXsample):
      derived_parameters(NXprocess):
      plot(NXdata):
```

plot(NXdata): Can be used to define a default figure for the main entry or any group of the application definition



General Metadata

```
(NXellipsometry):
  (NXentry):
    doc: |
      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:
      doc: "An application definition for ellipsometry."
      \@version:
        doc: "Version number to identify which definition of this application
          definition was used for this entry/data."
      \@url:
        doc: "URL where to find further material (documentation, examples)
          relevant to the application definition"
      enumeration: [NXellipsometry]

    experiment_identifier:
      doc: |
        Unique identifier of the experiment, such as a (globally persistent) unique
        identifier.
        i) The identifier is usually defined by the facility or principle investigator.
        ii) The identifier enables to link experiments to e.g. proposals.

    experiment_description:
      exists: recommended
      doc: "A free-text description of the experiment. What is the aim of the
        experiment? The general procedure."

    start_time(NX_DATE_TIME):
      doc: "Start time of the experiment. UTC offset should be specified."
```

```
    acquisition_program(NXprocess):
      exists: optional
      program:
        doc: "Commercial or otherwise defined given name to the program that was
          used to generate the result file(s) with measured data and metadata.
          This program converts the measured signals to ellipsometry data. If
          home written, one can provide the actual steps in the NOTE subfield
          here."
      version:
        doc: "Either version with build number, commit hash, or description of
          a (online) repository where the source code of the program and build
          instructions can be found so that the program can be configured in
          such a way that result files can be created ideally in a
          deterministic manner."
      \@url:
        doc: "Website of the software."

    (NXuser):
      exists: [min, 1]
      doc: "Contact information of at least the user of the instrument or the
        investigator who performed this experiment.
        Adding multiple users if relevant is recommended."
      name:
        doc: "Name of the user."
      affiliation:
        doc: "Name of the affiliation of the user at the point in time when the
          experiment was performed."
      address:
        doc: "Full address (street, street number, ZIP, city, country) of the
          user's affiliation."
      email:
        doc: "Email address of the user."
      orcid:
        exists: recommended
        doc: "Author ID defined by https://orcid.org/."
      telephone_number:
        exists: recommended
        doc: "Official telephone number of the user."
```

Ellipsometry Application Definition - INSTRUMENT

```
142   (NXinstrument):
143     doc: "General properties of the ellipsometry equipment"
144   > model: ···
149   > company: ···
152
153   > construction_year(NX_DATE_TIME): ···
157
158   > firmware: ···
165
166   > light_source(NXsource): ···
178
179   > focussing_probes(NX_BOOLEAN): ···
181
182   > data_correction(NX_BOOLEAN): ···
185
186   > angular_spread(NX_NUMBER): ···
190
191   > ellipsometry_type: ···
208
209   > calibration_status(NX_CHAR): ···
221
222   > calibration(NXsubentry): ···
295
296   > angle_of_incidence(NX_NUMBER): ···
303
304   > stage(NXsubentry): ···
345
346   > window(NXaperture): ···
408
409   > (NXdetector): ···
474
475   > spectrometer(NXmonochromator): ···
531
```

model: (required) NX_CHAR

The name of the instrument

@version: (required) NX_CHAR

The used version of the hardware if available. If not a commercial instrument use date of completion of the hardware.

company: (optional) NX_CHAR

Name of the company which build the instrument

construction_year: (optional) NX_DATE_TIME

ISO8601 date when the instrument was constructed. UTC offset should be specified.

firmware: (required) NX_CHAR

Commercial or otherwise defined name of the software that was used for the measurement

@version: (required) NX_CHAR

Version and build number or commit hash of the software source code

@url: (required) NX_CHAR

Website of the software.

Ellipsometry Application Definition - INSTRUMENT

```
142   (NXinstrument):
143     doc: "General properties of the ellipsometry equipment"
144   > model: ···
149   > company: ···
152
153   > construction_year(NX_DATE_TIME): ···
157
158   > firmware: ···
165
166   > light_source(NXsource): ···
178
179   > focussing_probes(NX_BOOLEAN): ···
181
182   > data_correction(NX_BOOLEAN): ···
185
186   > angular_spread(NX_NUMBER): ···
190
191   > ellipsometry_type: ···
208
209   > calibration_status(NX_CHAR): ···
221
222   > calibration(NXsubentry): ···
295
296   > angle_of_incidence(NX_NUMBER): ···
303
304   > stage(NXsubentry): ···
345
346   > window(NXaperture): ···
408
409   > (NXdetector): ···
474
475   > spectrometer(NXmonochromator): ···
531
```

ellipsometry_type: (required) NX_CHAR

What type of ellipsometry was used? See Fujiwara Table 4.2

Any of these values:

- `rotating analyzer`
- `rotating analyzer with analyzer compensator`
- `rotating analyzer with polarizer compensator`
- `rotating polarizer`
- `rotating compensator on polarizer side`
- `rotating compensator on analyzer side`
- `modulator on polarizer side`
- `modulator on analyzer side`
- `dual compensator`
- `phase modulation`
- `imaging ellipsometry`
- `null ellipsometry`

calibration_status: (required) NX_CHAR

Was a calibration performed? If yes, when was it done? If the calibration time is provided, it should be specified in calibration/calibration_time.

Any of these values:

- `calibration time provided`
- `no calibration`
- `within 1 hour`
- `within 1 day`
- `within 1 week`

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```
142   (NXinstrument):
143     doc: "General properties of the ellipsometry equipment"
144   > model: ···
149   > company: ···
152
153   > construction_year(NX_DATE_TIME): ···
157
158   > firmware: ···
165
166   > light_source(NXsource): ···
178
179   > focussing_probes(NX_BOOLEAN): ···
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182   > data_correction(NX_BOOLEAN): ···
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186   > angular_spread(NX_NUMBER): ···
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296   > angle_of_incidence(NX_NUMBER): ···
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304   > stage(NXsubentry): ···
345
346   > window(NXaperture): ···
408
409   > (NXdetector): ···
474
475   > spectrometer(NXmonochromator): ···
531
```

DETECTOR: (required) NXdetector

Which type of detector was used, and what is known about it? A detector can be a photomultiplier (PMT), a CCD in a camera, or an array in a spectrometer. If so, the whole detector unit goes in here. Integration time is the count time field, or the real time field. See their definition.

detector_type: (required) NX_CHAR

What kind of detector module is used, e.g. CCD-spectrometer, CCD camera, PMT, photodiode, etc.

Any of these values:

- `PMT`
- `photodiode`
- `avalanche diode`
- `CCD camera`
- `CCD spectrometer`
- `other`

other_detector: (optional) NX_CHAR

If you specified ‘other’ as detector type, please write down what it is.

revolution: (optional) NX_NUMBER {units=NX_ANY}

Define how many rotations of the rotating element were taken into account per spectrum.

Ellipsometry Application Definition - SAMPLE

```
(NXsample):
  doc: "Properties of the sample, its history, the sample environment
    and experimental conditions (e.g. surrounding medium, temperature,
    pressure etc.), along with the data (data type, wavelength array,
    measured data)."
  atom_types: ···
  sample_name: ···

  sample_history: ···

  preparation_date(NX_DATE_TIME): ···

  layer_structure: ···

  data_identifier(NX_NUMBER): ···

  data_type: ···

  column_names: ···

  measured_data(NX_NUMBER): ···

  data_error(NX_NUMBER): ···

  time_points(NX_NUMBER): ···

  environment_conditions(NXenvironment): ···
```

data_type: (required) NX_CHAR

Select which type of data was recorded, for example Psi and Delta (see: https://en.wikipedia.org/wiki/Ellipsometry#Data_acquisition). It is possible to have multiple selections. Data types may also be converted to each other, e.g. a Mueller matrix contains N,C,S data as well. This selection defines how many columns (N_variables) are stored in the data array.

Any of these values:

- `psi/delta`
- `tan(psi)/cos(delta)`
- `Mueller matrix`
- `Jones matrix`
- `N/C/S`
- `raw data`

column_names: (required) NX_CHAR (Rank: 1, Dimensions: [N_variables])

Please list in this array the column names used in your actual data. That is ['psi', 'delta'] or ['MM1', 'MM2', 'MM3', …, 'MM16] for a full Mueller matrix, etc.

measured_data: (required) NX_NUMBER (Rank: 5, Dimensions: [N_time, N_p1, N_angles, N_variables, N_wavelength])

Resulting data from the measurement, described by data type. Minimum two columns containing Psi and Delta, or for the normalized Mueller matrix it may be 16 (or 15 if the element (1,1) is all 1).

Ellipsometry Application Definition - SAMPLE

```
(NXsample):
  doc: "Properties of the sample, its history, the sample environment
    and experimental conditions (e.g. surrounding medium, temperature,
    pressure etc.), along with the data (data type, wavelength array,
    measured data)."
  atom_types: ···
  sample_name: ···

  sample_history: ···

  preparation_date(NX_DATE_TIME): ···

  layer_structure: ···

  data_identifier(NX_NUMBER): ···

  data_type: ···

  column_names: ···

  measured_data(NX_NUMBER): ···

  data_error(NX_NUMBER): ···

  time_points(NX_NUMBER): ···

  environment_conditions(NXenvironment): ···
```

```
environment_conditions(NXenvironment):
  doc: "Specify external parameters that have influenced the sample."

  medium:
    doc: "Describe what was the medium above or around the sample. The
      common model is built up from the substrate to the medium on the
      other side. Both boundaries are assumed infinite in the model.
      Here, define the name of the medium (e.g. water, air, UHV, etc.)."

  medium_refractive_indices(NX_NUMBER): ···

  number_of_runs(NX_UINT): ···

  varied_parameters: ···

  optical_excitation(NXsource):
    exists: optional
    doc: ···

    wavelength(NX_NUMBER): ···

    broadening(NX_NUMBER): ···

    duration(NX_NUMBER): ···

    pulse_energy(NX_NUMBER): ···

  (NXsensor):
    exists: optional
    doc: "A sensor used to monitor an external condition. The value
      field contains the measured values. If it is constant within
      an error for every run then use only an array of length one."
```

Questions or Comments?

- If you have questions regarding the ellipsometry application definition, please feel free to contact us:
  Carola Emminger: emminger.carola@physik.hu-berlin.de
  Chris Sturm: csturm@physik.uni-leipzig.de
- You can also leave comments at https://fairmat-experimental.github.io/nexus-fairmat-proposal/1c3806dba40111f36a16d0205cc39a5b7d52ca2e/classes/contributed_definitions/NXellipsometry.html#nxellipsometry

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