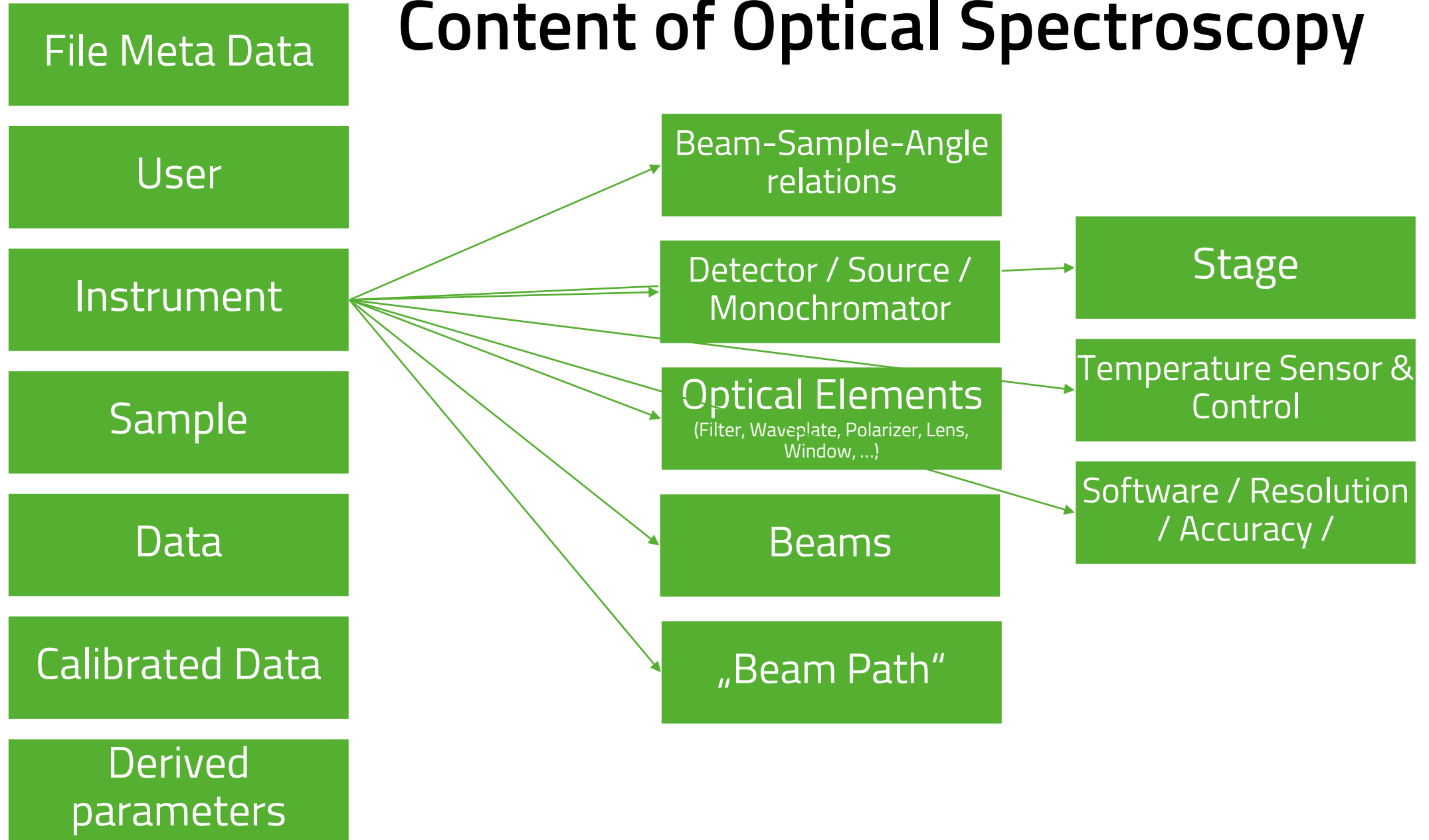





Optical Spectroscopy

NeXus definition & it's content

Content of Optical Spectroscopy



File Meta Data

- NeXus definition → Version+URL
- Title: Silicon-Substrate-111
- Start/End time: 2020-07-10 15:00:00+2
- Description of experiment type: (time-resolved) Raman/Ellipsometry
- Identifier: I  **Foundation**
- Reference frames: *What coordinate systems you want to use*

AND

2.3.3.3.183. NXopt

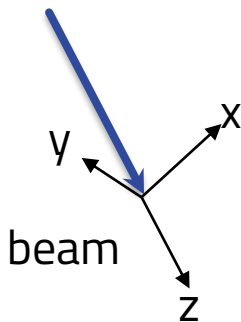
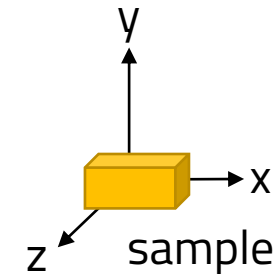
Structure:

ENTRY: (required) [NXentry](#)


definition: (required) [NX_CHAR](#) ⇐

► An application definition describing a general optical experiment. ...

Options: (required) [NX_CHAR](#)



File Meta Data

- NeXus definition → Version 2.3.3.1.17. NXentry
- Title: Silicon-Substrate-1
- Start/End time: 2020-07-14 12:00:00 - 2020-07-14 12:00:00
- Description of experiment: X-ray reflectivity measurement of a silicon substrate
- Identifier:  **Foundation**
- Reference frames: *What coordinate system to use*

2.3.3.1.17. NXentry

Status:
base class extends [NXobject](#)

Description:
▶ (**required**) :ref:`NXentry` describes the measurement ...

Symbols:
No symbol table

Groups cited:
[NXcollection](#), [NXdata](#), [NXinstrument](#), [NXmonitor](#), [NXnote](#), [NXprocessor](#)

Structure:

@default: (optional) [NX_CHAR](#)
▶ Declares which :ref:`NXdata` group contains the data ...

@IDF_Version: (optional) [NX_CHAR](#)
ISIS Muon IDF_Version

title: (optional) [NX_CHAR](#)
Extended title for entry

experiment_identifier: (optional) [NX_CHAR](#)
▶ Unique identifier for the experiment, ...

experiment_description: (optional) [NX_CHAR](#)
Brief summary of the experiment, including key objectives.

collection_identifier: (optional) [NX_CHAR](#)

man/Ellipsometry

AND

2.3.3.3.183. NXopt

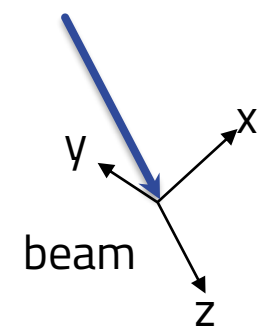
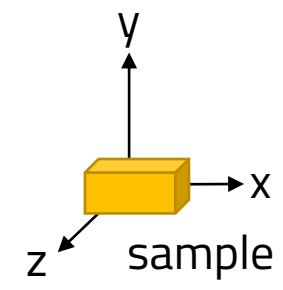
Structure:

ENTRY: (required) [NXentry](#)

definition: (required) [NX_CHAR](#) ⇐

▶ An application definition describing a general optical experiment. ...

nt to use



User

- Name
- Role
- Affiliation
- Address
- Telephone number
- Mail
- ID

In NXopt (i.e. thats all!):

USER: (optional) [NXuser](#) ⇌

▼ Contact information and eventually details of at persons who ...

Contact information and eventually details of at persons who perform
Examples are: name, affiliation, address, telephone number, email, 1
users if relevant.

Due to data privacy concerns, there is no minimum requirement.

In NXuser:

Structure:

@default: (optional) [NX_CHAR](#)

► Declares which child group contains a path leading ...

name: (optional) [NX_CHAR](#)

Name of user responsible for this entry

role: (optional) [NX_CHAR](#)

► Role of user responsible for this entry. ...

affiliation: (optional) [NX_CHAR](#)

Affiliation of user

address: (optional) [NX_CHAR](#)

Address of user

telephone_number: (optional) [NX_CHAR](#)

Telephone number of user

fax_number: (optional) [NX_CHAR](#)

Fax number of user

email: (optional) [NX_CHAR](#)

Email of user

facility_user_id: (optional) [NX_CHAR](#)

► facility based unique identifier for this person ...

IDENTIFIER: (optional) [NXidentifier](#)

► Details about an author code, open researcher, or contributor .

File Meta Data

User

Instrument

Sample

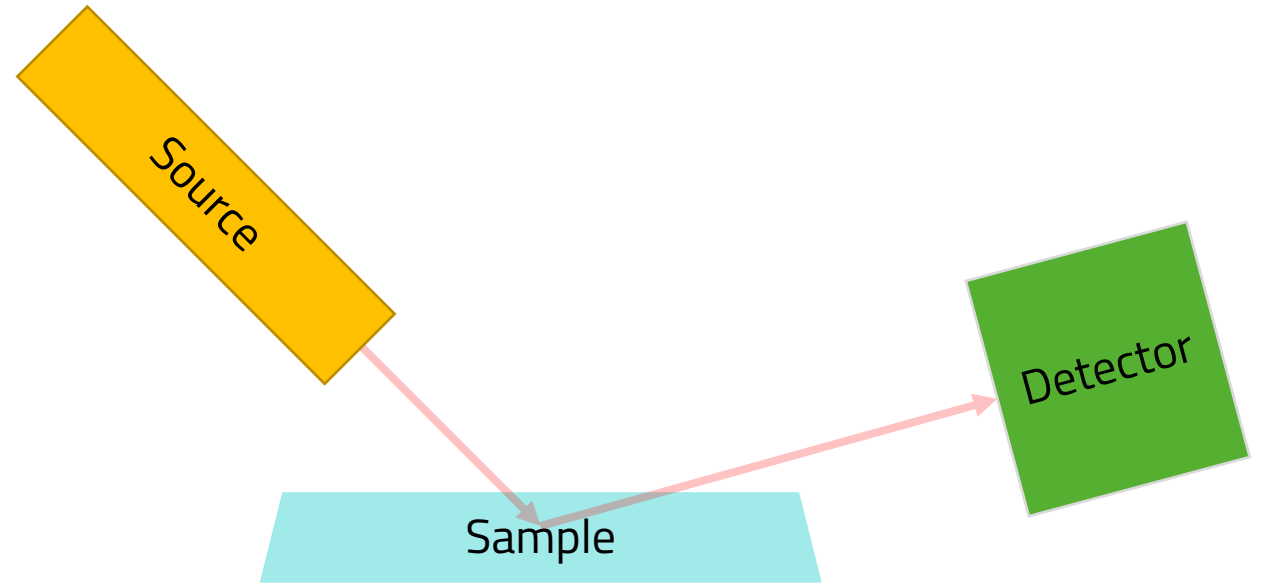
Data

Calibrated Data

Derived
parameters



Instrument



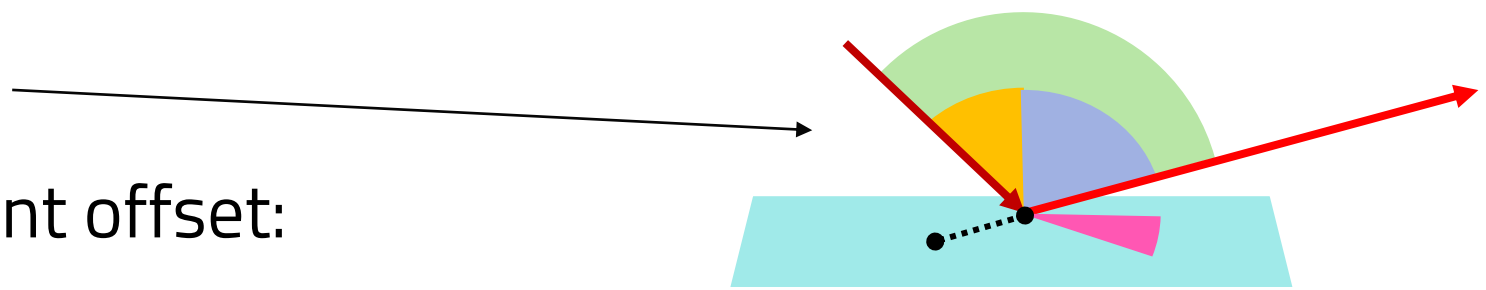
"A general optical experiment consists of (i) a light/photon source, (ii) a sample, (iii) a detector."

Photon-in, photon-out → (ellipsometry, Raman, photoluminescence, reflectivity/transmission spectroscopy).

→ No electrons, no chemoluminescence, ...



Instrument #1

- Reference frame for angles: Sample or Beam centered
- Angles: A diagram illustrating an instrument setup. A light blue trapezoidal sample is shown. A red arrow representing a beam is incident on the sample surface. A dashed line indicates the focal point offset. A green arc represents the angular range. A yellow sector is shown between the incident beam and a vertical reference line. A blue sector is shown between the vertical reference line and a pink sector. A black arrow points from the text 'Angles:' to the yellow sector.
- Focal point offset:
- Medium refractive index: „n=1.33“
- Device information → vendor, model, ID, constr.-year
- Software_TYPE: LabSpec.exe v1.23.45
- Resolution: 5pm
- Device calibration → Method, Status, Time, Accuracy, Link-to-file

File Meta Data

User

Instrument

Sample

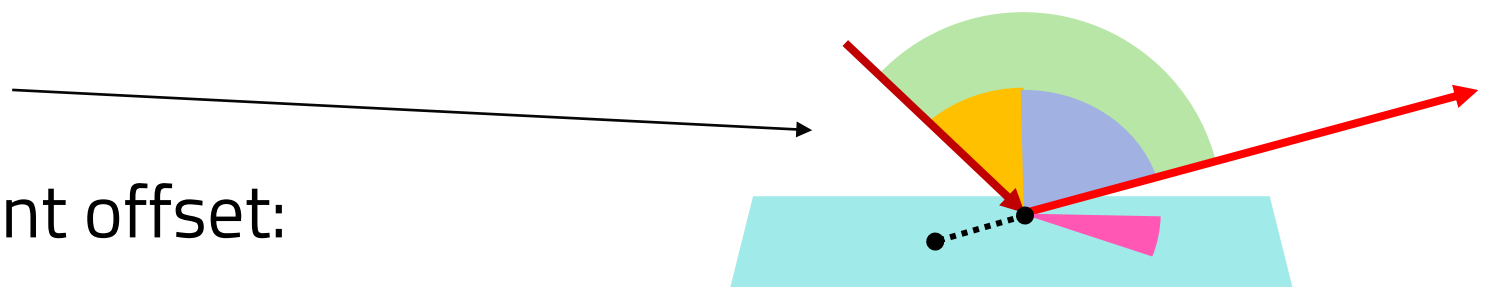
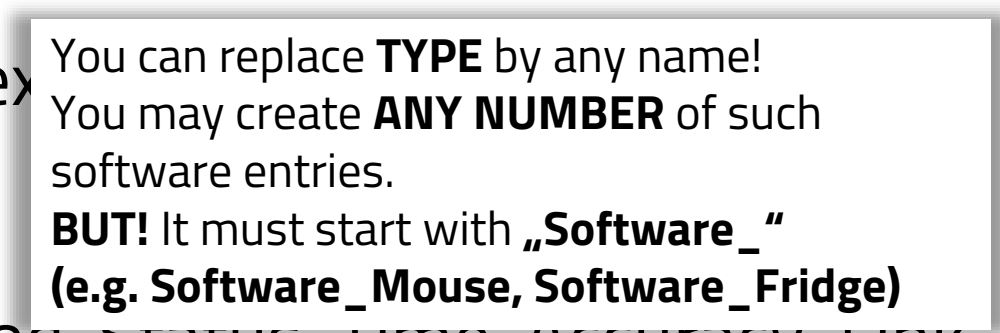
Data

Calibrated Data

Derived parameters



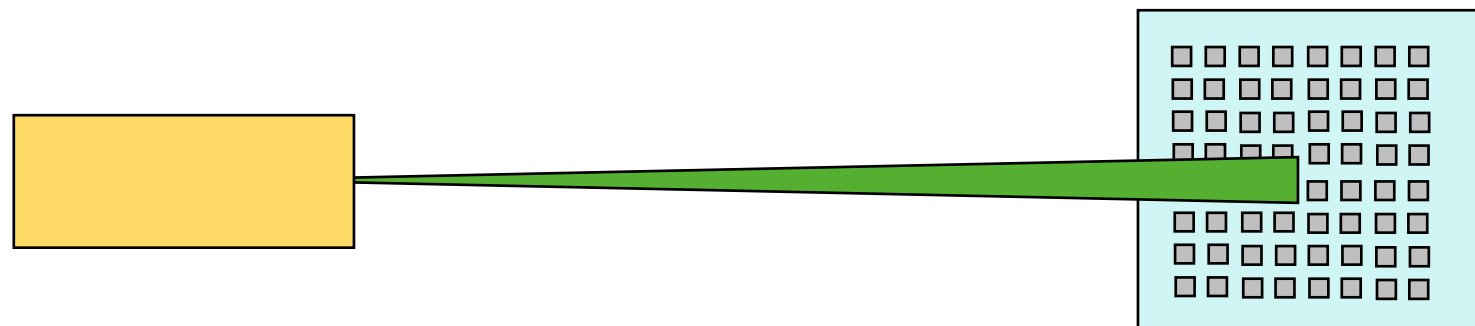
Instrument #1

- Reference frame for angles: Sample or Beam centered
- Angles: A diagram showing a light blue trapezoidal sample. A red arrow (beam) enters from the top left, hits the top surface, and reflects as another red arrow exiting to the top right. A black dot on the top surface is connected to a black dot on the bottom surface by a dotted line. Colored sectors (yellow, blue, pink, green) are shown around the top surface, representing different angular regions. A black arrow points from the text 'Angles:' to the diagram.
- Focal point offset:
- Medium refractive index: „n=1.33“
- Device information → vendor, model, ID, constr.-year
- Software **TYPE:** LabSpec.exe A white callout box with a grey border containing text: 'You can replace **TYPE** by any name! You may create **ANY NUMBER** of such software entries. **BUT!** It must start with „**Software_**“ (e.g. **Software_Mouse**, **Software_Fridge**)'. A red arrow points from the 'TYPE:' text in the list item to the callout box.
- Resolution: 5pm
- Device calibration → Method, Status, Time, Accuracy, Link-to-file



Instrument #2

- **Beam_TYPE** → Wavelength, Size, Spread, Divergence, Polarization, Power, : 532nm, 100mW, 0.1°, 3mm, linear,
- Beam-Transfer-Matrices
- **Source_TYPE** → type, name, device information & characteristics, associated beam
- **Detector_TYPE** → similar to Source + raw_data

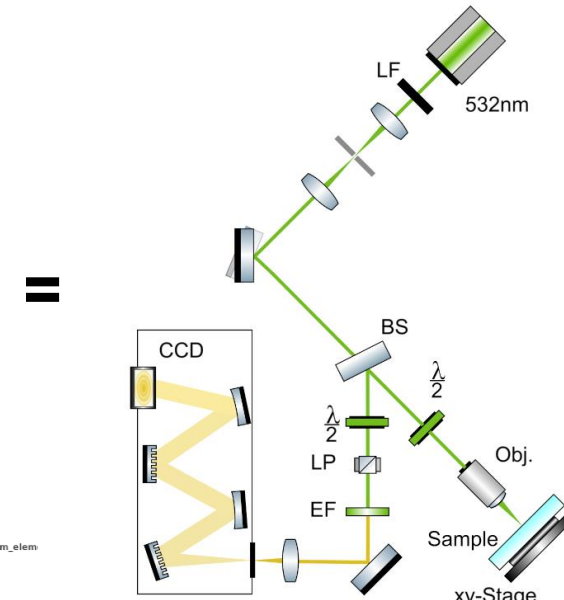
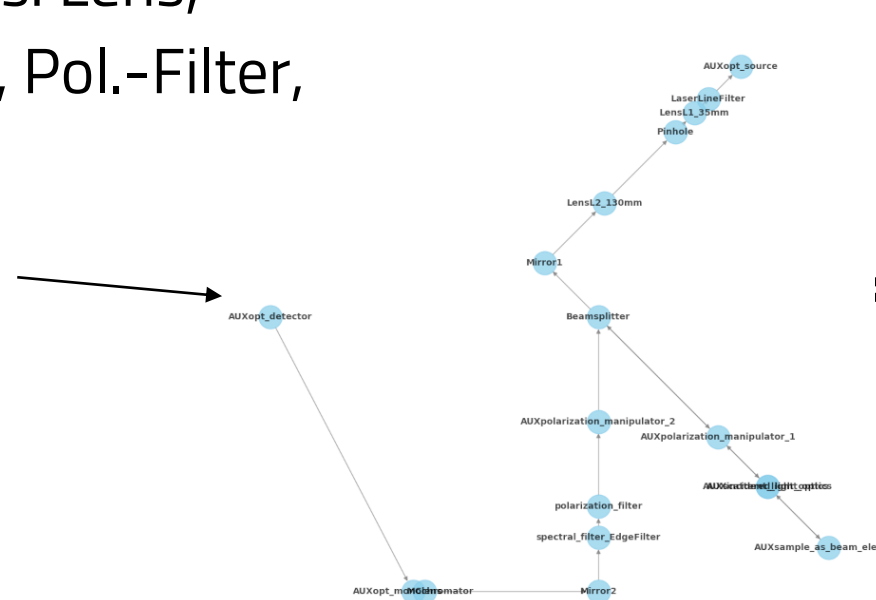


Instrument #3



File Meta Data
User
Instrument
Sample
Data
Calibrated Data
Derived parameters

- Monochromators → Characteristics + NXmonochromator: wavelength/energy + errors, intensity distribution, grating
- Various optical elements: Lens, Waveplates, Windows, Pol.-Filter, Spectral-Filter
- „Beam Path Devices“
- Sample Stage
- Temperatur Sensor
- Temperatur Controller

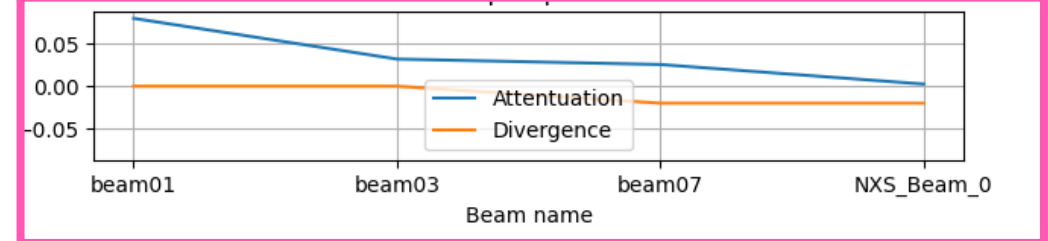
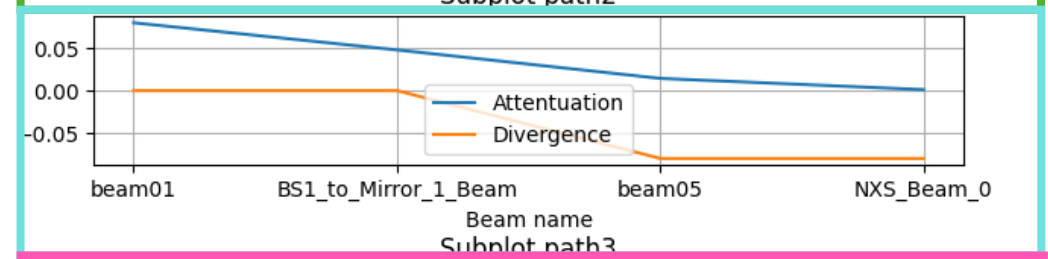
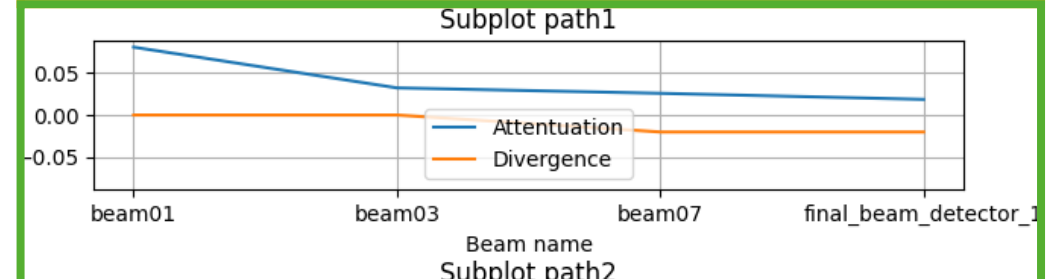
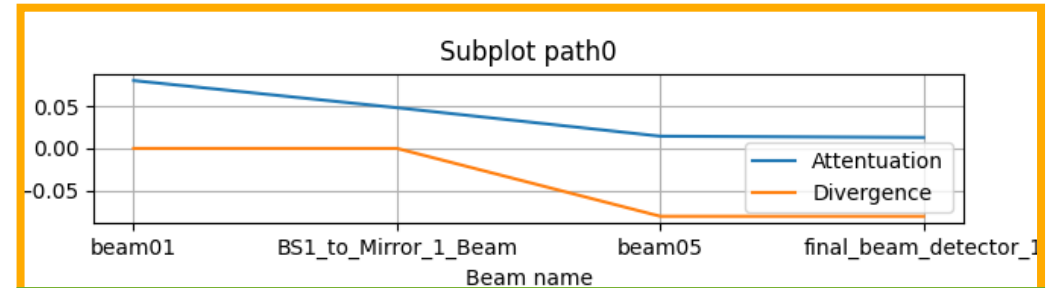
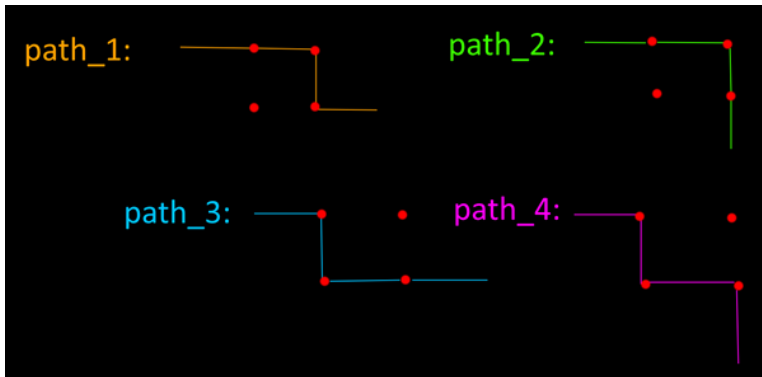
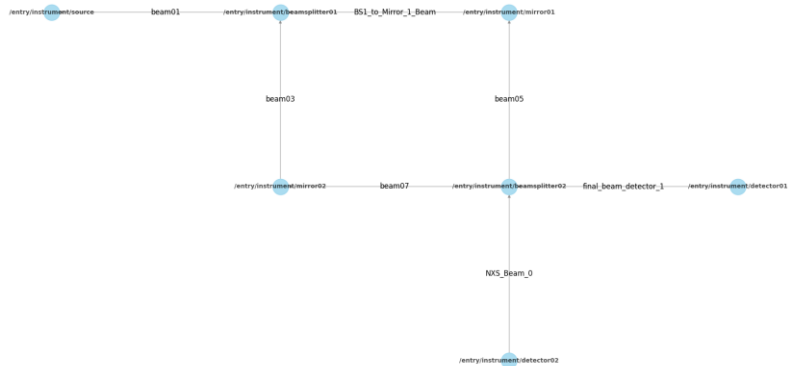
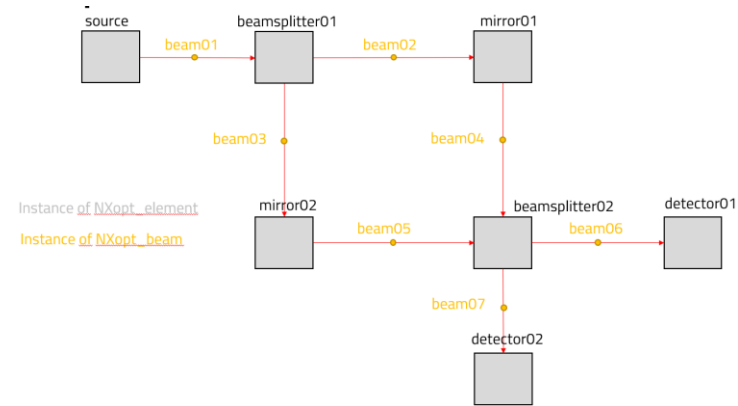


AND

Everything in NXinstrument

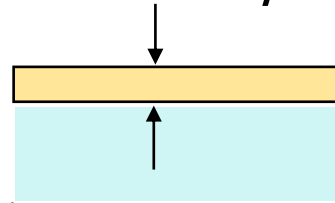
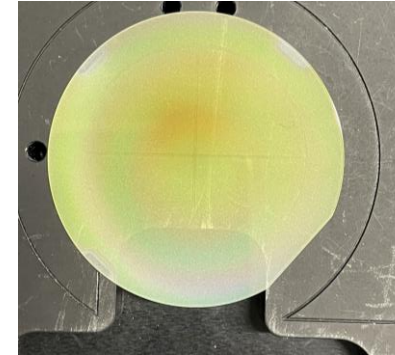
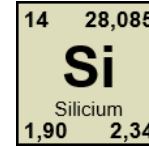


Instrument #4 → „Beam Path Devices“



Sample

- Name, ID, description
- Chem. Elements / Formula
- Form: single crystal, thin film, multi-layer,
- Thickness
- Layer Structure / Substrate
- History (Processing/deposition steps)
- Temperature → link to Sensor
- Environment / External parameters



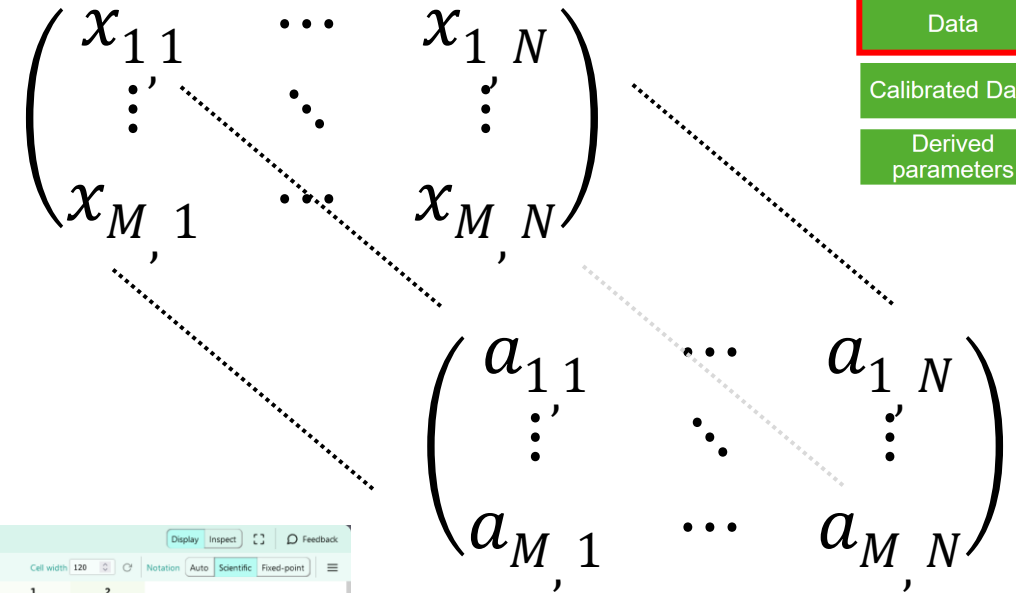
- temperature
- pH
- magnetic_field
- electric_field
- current
- conductivity
- resistance
- voltage
- pressure
- flow
- stress
- strain
- shear
- surface_pressure

- File Meta Data
- User
- Instrument
- Sample**
- Data
- Calibrated Data
- Derived parameters

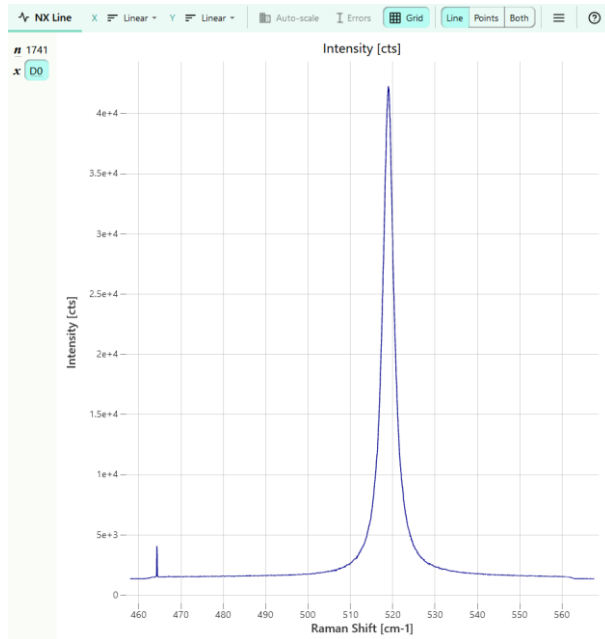


Data

- Defines „default plot“
- Can stores ANY data
- Link to data entries
- Assignment of axis types



- File Meta Data
- User
- Instrument
- Sample
- Data**
- Calibrated Data
- Derived parameters



#	3	2	1088	0	1	2
x	D0	D1	D2	4.001e+1	3.828e+1	3.736e+1
y	D0	D1	D2	4.003e+1	3.829e+1	3.733e+1
				4.003e+1	3.827e+1	3.727e+1
				4.005e+1	3.826e+1	3.725e+1
				4.007e+1	3.826e+1	3.723e+1
				4.008e+1	3.825e+1	3.721e+1
				4.008e+1	3.825e+1	3.717e+1
				4.008e+1	3.825e+1	3.712e+1
				4.007e+1	3.821e+1	3.706e+1
				4.007e+1	3.820e+1	3.702e+1
				4.007e+1	3.819e+1	3.696e+1
				4.007e+1	3.815e+1	3.690e+1
				4.006e+1	3.813e+1	3.684e+1
				4.006e+1	3.811e+1	3.677e+1
				4.004e+1	3.807e+1	3.670e+1
				4.002e+1	3.804e+1	3.665e+1
				4.003e+1	3.802e+1	3.662e+1
				4.003e+1	3.799e+1	3.655e+1
				4.001e+1	3.798e+1	3.648e+1
				4.001e+1	3.796e+1	3.643e+1
				4.001e+1	3.793e+1	3.638e+1
				4.000e+1	3.792e+1	3.633e+1
				4.000e+1	3.791e+1	3.629e+1
				4.000e+1	3.789e+1	3.624e+1
				4.000e+1	3.788e+1	3.618e+1
				4.000e+1	3.787e+1	3.614e+1
				4.000e+1	3.786e+1	3.611e+1
				4.000e+1	3.785e+1	3.605e+1



Calibrated Data

- Contains mathematical mapping/processing of raw-data: $\lambda_{\text{uncalib}} \rightarrow \lambda_{\text{calib}}$

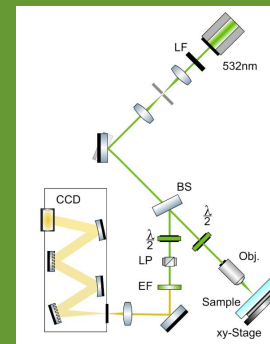
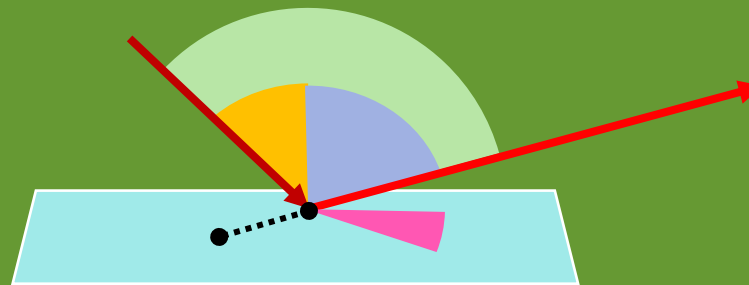
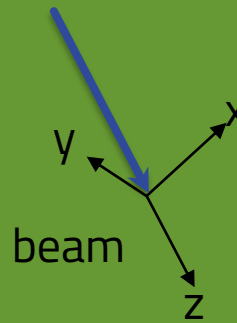
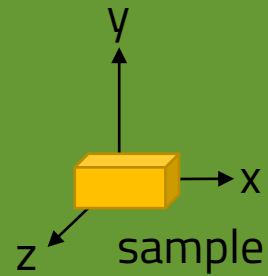
Derived parameters

- Results of a mathematical data processing: depolarization, reflectivity, peak parameters, refractive index, absorption coefficient, coupling strength,
- ANALYSIS_program
- Will be updated later...





NXopt



$$\begin{pmatrix} x_{1,1} & \dots & x_{1,N} \\ \vdots & \ddots & \vdots \\ x_{M,1} & \dots & x_{M,N} \end{pmatrix}
 \begin{pmatrix} a_{1,1} & \dots & a_{1,N} \\ \vdots & \ddots & \vdots \\ a_{M,1} & \dots & a_{M,N} \end{pmatrix}$$

File Meta Data
User
Instrument
Sample
Data
Calibrated Data
Derived parameters

