# **Multidimensional photoemission spectroscopy metadata parameters**

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Description and compatibility with existent Nexus structures. This is done with the approach of NeXus base classes, i.e. to develop the maximally wide set of possible parameters for the broadest reach in the ARPES community. Ideally, this could be the list from which an autocompletion algorithm could draw when building NeXus files for the ARPES community.

In general, we tried to avoid “bending the purpose” of a grouping. We favoured creating a new group with precise and descriptive character rather than appending a parameter to an existing category clearly meant for something else.

**Legend**

|  |  |
| --- | --- |
|  | **Not present in NeXus or NXarpes hierarchy – added by Max Planck** |
|  | **Not present in NeXus or NXarpes hierarchy – added by APE** |
|  | **Present in NeXus hierarchy** |
|  | **Present in NXarpes hierarchy, not in NeXus** |
| **v** | **Present in the NXarpes required list** |
| **x** | **Absent from NXarpes required list** |

Where needed, the new parts of the hierarchy are marked in red.

**General Parameters**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Name | Unit | Description | Nexus hierarchy | NX variable | NXarpes |
| experiment\_title | None | Title of the experiment | NXentry:experiment\_title | NX\_CHAR | **x** |
| experiment\_location | None | City and country where ex. Took place | NXentry:experiment\_location | NX\_CHAR | **x** |
| experiment\_geotag | Degrees | Geographical coordinates of the place. Necessary when converting data with naïve dates. | NXentry:experiment\_geotag | NX\_FLOAT:NX\_ANGLE | **x** |
| experiment\_start\_date | None | Start date and time of ex. in ISO 8601 format, ideally including UTC offset. | NXentry:experiment\_start\_date | NX\_DATE\_TIME | **x** |
| experiment\_start\_date\_timestamp | Seconds | Machine readable, absolute timestamp using UNIX epoch. | NXentry:experiment\_start\_date\_timestamp | NX\_FLOAT:NX\_TIME | **x** |
| experiment\_end\_date | None | Start date and time of ex. in ISO 8601 format, ideally including UTC offset. | NXentry:experiment\_end\_date | NX\_DATE\_TIME | **x** |
| experiment\_end\_date\_timestamp | Seconds | Machine readable, absolute timestamp using UNIX epoch. | NXentry:experiment\_start\_date\_timestamp | NX\_FLOAT:NX\_TIME | **x** |
| experiment\_summary | None | Descriptive summary of ex. | NXentry:experiment\_description  NXentry:experiment\_documentation | NX\_CHAR | **x** |
| experiment\_identifier | None | Unique identifier for the experiment. | NXentry:experiment\_identifier | NX\_CHAR | **x** |
| experiment\_run\_cycle | None | Some facilities organize their beamtime into run cycles. | NXentry:run\_cycle | NX\_CHAR | **x** |
| experiment\_institution | None | Name of the institution hosting the facility | NXentry:experiment\_institution | NX\_CHAR | **x** |
| experiment\_facility | None | Name of the experimental facility | NXentry:experiment\_facility | NX\_CHAR | **x** |
| experiment\_laboratory | None | Name of the laboratory or beamline | NXentry:experiment\_laboratory | NX\_CHAR | **x** |

**Entry specific parameters**

An entry is meant to be relative to a single “measurement” i.e. it contains data and metadata relative to an acquisition of a specific observable.

Some of the parameters in the original list are present in the NeXus hierarchy, but much deeper in the tree. If it is decided that these parameters are necessary at this point in the hierarchy, they could be still saved in positions following the NX standard, but cross-linked in a freeform general field called NXentry:notes.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Name | Unit | Description | Nexus hierarchy | NX variable | NXarpes |
| entry\_title | None | Title of the entry, referring to a specific measurement. | NXentry: title | NX\_CHAR | **v** |
| entry\_identifier | None | Identifier of the measurement | NXentry:entry\_identifier | NX\_CHAR | **x** |
| entry\_start\_time | Date | Start date and time of ex. in ISO 8601 format, ideally including UTC offset. | NXentry: start\_time | NX\_DATE\_TIME | **v** |
| entry\_start\_date\_timestamp | Seconds | Machine readable, absolute timestamp using UNIX epoch. | NXentry:entry\_start\_date\_timestamp | NX\_FLOAT:NX\_TIME | **x** |
| entry\_end\_time | Date | Ending date of the measurement | NXentry: end\_time | NX\_DATE\_TIME | **x** |
| entry\_end\_date\_timestamp | Seconds | Machine readable, absolute timestamp using UNIX epoch. | NXentry:entry\_end\_date\_timestamp | NX\_FLOAT:NX\_TIME | **x** |
| entry\_duration | s | Duration of the measurement | NXentry: duration | NX\_FLOAT:NX\_TIME | **x** |
| entry\_collection\_time | s | Time spent actually collecting data | NXentry:collection\_time | NX\_FLOAT:NX\_TIME | **x** |
| definition | None | Does the file correspond to a standardized structure? | NXentry:definition | NX\_CHAR | **v**  **NXarpes** |

**User parameters**

Information about the user responsible for the entry is significant. It is also well organized in NeXus hierarchy.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Name | Unit | Description | Nexus hierarchy | NX variable | NXarpes |
| name | none | Name of user responsible for this entry | NXentry:NXuser:name | NX\_CHAR | **x** |
| role | none | Role of user (local contact, principal investigator, etc.) | NXentry:NXuser:role | NX\_CHAR | **x** |
| affiliation | none | Affiliation of user | NXentry:NXuser:affiliation | NX\_CHAR | **x** |
| address | none | Address of user | NXentry:NXuser:address | NX\_CHAR | **x** |
| telephone\_number | none | Telephone number of user | NXentry:NXuser:telephone\_number | NX\_CHAR | **x** |
| email | none | E-mail address of user | NXentry:NXuser:email | NX\_CHAR | **x** |
| facility\_user\_id | none | User identifier defined by the facility | NXentry:NXuser:facility\_user\_id | NX\_CHAR | **x** |
| ORCID | none | ORCID of the user | NXentry:NXuser:ORCID | NX\_CHAR | **x** |

**Instrumentation parameters**

The class NXinstrument refers to the whole set-up (beamline, or apparatus in a lab), and the sub-components are defined within it as sub-groups.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Name | Unit | Description | Nexus hierarchy | NX variable | NXarpes |
| instrument\_name | None | Name or model of the equipment | NXentry:NXinstrument:name  attribute:@short\_name (acronym) | NX\_CHAR | **x** |
| instrument\_temporal\_resolution | fs | Overall time resolution (FWHM of cross correlation) | NXentry:NXinstrument:temporal\_resolution | NX\_FLOAT:NX\_TIME | **x** |
| instrument\_energy\_resolution | eV | Overall energy resolution (FWHM of gaussian broadening) | NXentry:NXinstrument:energy\_resolution | NX\_FLOAT:NX\_ENERGY | **x** |
| instrument\_spatial\_resolution | um | Overall spatial resolution (Airy disk radius) | NXentry:NXinstrument:spatial\_resolution | NX\_FLOAT:NX\_LENGTH | **x** |
| instrument\_description | None | Short description of the instrument, possibly reference to a technical publication | NXentry:NXinstrument:description | NX\_CHAR | **x** |

**Source information**

NXsource is the group class that refers to the properties of the instrument that generates the beam. For the properties of the beam at the sample position, see NXbeam. In a pump and probe experiment the probe can be called as source:NXsource and the pump as source\_pump:NXsource without creating ambiguity. The most relevant scope of the source class is to describe things like time structure of the source, or to store source related diagnostics (beam current in a synchrotron, power monitors in a laser source, etc.). In the worked example some further parameters are created to deal with the especially complex timestructure of FLASH.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Name | Unit | Description | Nexus hierarchy | NX variable | NXarpes |
| name | None | Name of the source | NXentry:NXinstrument:NXsource:name (@short\_name) | NX\_CHAR | **v** |
| type | None | Type of radiation source | NXentry:NXinstrument:NXsource:type[[1]](#footnote-1) | NX\_CHAR | **v** |
| probe | None | Type of radiation used as probe | NXentry:NXinstrument:NXsource:probe[[2]](#footnote-2) | NX\_CHAR | **v**  **x-ray** |
| photon\_energy | eV | The center photon energy of the source, before it is monochromatized or converted | NXentry:NXinstrument:NXsource:photon\_energy | NX\_FLOAT:NX\_ENERGY | **x** |
| center\_wavelength | nm | The center wavelength of the source, before it is monochromatized or converted | NXentry:NXinstrument:NXsource:center\_wavelength | NX\_FLOAT:NX\_WAVELENGTH | **X** |
| pulse\_energy | uJ | For pulsed sources, the energy of a single pulse | NXentry:NXinstrument:NXsource:pulse\_energy | NX\_FLOAT:NX\_ENERGY | **x** |
| peak\_power | W | For pulsed sources, the pulse energy divided by the pulse duration | NXentry:NXinstrument:NXsource:peak\_power | NX\_FLOAT:NX\_POWER | **x** |
| average\_power | W | Source power | NXentry:NXinstrument:NXsource:average\_power | NX\_FLOAT:NX\_POWER | **x** |
| emittance\_x | nm-rad | Horizontal emittance | NXentry:NXinstrument:NXsource:emittance\_x | NX\_FLOAT:NX\_EMITTANCE | **x** |
| emittance\_y | nm-rad | Vertical emittance | NXentry:NXinstrument:NXsource:emittance\_y | NX\_FLOAT:NX\_ EMITTANCE | **x** |
| size\_x | um | horizontal beam size | NXentry:NXinstrument:NXsource:sigma\_x | NX\_FLOAT:NX\_LENGTH | **x** |
| size\_y | um | vertical beam size | NXentry:NXinstrument:NXsource:sigma\_y | NX\_FLOAT:NX\_LENGTH | **x** |
| flux | s-1cm-2 | Photon flux of the source | NXentry:NXinstrument:NXsource:flux | NX\_FLOAT:NX\_FLUX | **x** |
| energy | J | Particle beam energy/excitation voltage | NXentry:NXinstrument:NXsource:energy | NX\_FLOAT:NX\_ENERGY | **x** |
| current | A | Storage ring current/X-ray tube current | NXentry:NXinstrument:NXsource:current | NX\_FLOAT:NX\_CURRENT | **x** |
| repetition\_rate | Hz | Pulsed source frequency (repetition rate) | NXentry:NXinstrument:NXsource:frequency | NX\_FLOAT:NX\_FREQUENCY | **x** |
| pulse\_duration | ps | Duration of the source pulses | NXentry:NXinstrument:NXsource:pulse\_width | NX\_FLOAT:NX\_TIME | **x** |
| spectrum | nm-1 or eV-1 | Energy/wavelength spectrum of the source | NXentry:NXinstrument:NXsource:distribution | NX\_FLOAT:NXdata | **x** |
| number\_of\_bunches | None | Number of bunches in the storage ring | NXentry:NXinstrument:NXsource:number\_of\_bunches | NX\_INT | **x** |
| bunch\_length | ps | Temporal length of the bunch | NXentry:NXinstrument:NXsource:bunch\_length | NX\_FLOAT:NX\_TIME | **x** |
| bunch\_distance | ns | Time between bunches | NXentry:NXinstrument:NXsource:bunch\_distance | NX\_FLOAT:NX\_TIME | **x** |
| mode | None | Source operating mode (single or multi bunch) | NXentry:NXinstrument:NXsource:mode | NX\_CHAR | **x** |
| top\_up | Bool | Is the storage ring in top up? | NXentry:NXinstrument:NXsource:top\_up | NX\_BOOLEAN | **x** |
| bunch\_structure | s-1 | Description of the bunch pattern | NXentry:NXinstrument:NXsource:bunch\_pattern | NX\_FLOAT:NXdata | **x** |
| rms\_jitter | fs | For pump-probe experiments, the synchronization error between pump and probe. | NXentry:NXinstrument:NXsource:rms\_jitter | NX\_FLOAT:NX\_TIME | **x** |
| bunch\_number\_start | None | Some facilities tag each bunch. First bunch of the measurement | NXentry:NXinstrument:NXsource:bunch\_number\_start | NX\_INT | **x** |
| bunch\_number\_end | None | Last bunch of the measurement | NXentry:NXinstrument:NXsource:bunch\_number\_end | NX\_INT | **x** |

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**Beam**

NXbeam allows to specify the properties of the beam at any desired point of the beamline. Its most important use is to define the properties at the sample. We propose to use the naming convention: beam\_probe\_0 for the properties of the probe beam at the sample. In case a pump is present, we propose to use beam\_pump\_0. If there is reason to include in the metadata the beam properties at other points, we propose to increase the last number, either sequentially (0,1,2,...) or according to the distance from the sample in cm.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Name** | **Unit** | **Description** | **Nexus hierarchy** | **NX variable** | **NXarpes** |
| distance | cm | Distance from the sample | NXentry:NXinstrument:NXbeam:distance | NX\_FLOAT:NX\_LENGTH | **x** |
| pulse\_energy | uJ | Energy of a single pulse at the sample | NXentry:NXinstrument:NXbeam:pulse\_energy | NX\_FLOAT:NX\_ENERGY | **x** |
| average\_power | W | Average power at the sample | NXentry:NXinstrument:NXbeam:average\_power | NX\_FLOAT:NX\_POWER | **x** |
| photon\_energy | eV | The center photon energy at sample | NXentry:NXinstrument:NXbeam:photon\_energy | NX\_FLOAT:NX\_ENERGY | **x** |
| polarization\_angle | Deg | Angle of polarization ellipse from the plane of incidence. NaN for circular. | NXentry:NXinstrument:NXbeam:polarization\_angle | NX\_FLOAT:NX\_ANGLE | **x** |
| polarization\_ellipticity | None | Ellipticity of polarization, [-1,1]. | NXentry:NXinstrument:NXbeam:polarization\_ellipticity | NX\_FLOAT | **x** |
| size\_x | um | horizontal beam size | NXentry:NXinstrument:NXbeam:size\_x | NX\_FLOAT:NX\_LENGTH | **x** |
| size\_y | um | vertical beam size | NXentry:NXinstrument:NXbeam:size\_y | NX\_FLOAT:NX\_LENGTH | **x** |
| fluence | mJ cm-2 | Incident fluence at the sample | NXentry:NXinstrument:NXbeam:fluence | NX\_FLOAT:NX\_ANY | **x** |
| pulse\_duration | ps | Duration of the pulses at the sample | NXentry:NXinstrument:NXbeam:pulse\_duration | NX\_FLOAT:NX\_TIME | **x** |
| chirp\_spectrum | fs-1 | Spectrum of pulse frequency vs time. | NXentry:NXinstrument:NXbeam:chirp\_spectrum | NX\_FLOAT:NX\_Data | **x** |
| chirp\_type | none | The type of chirp implemented | NXentry:NXinstrument:NXbeam:chirp\_type | NX\_CHAR | **x** |
| chirp\_GDD | fs2 | Group delay dispersion of the pulse for linear chirp | NXentry:NXinstrument:NXbeam:chirp\_GDD | NX\_FLOAT:NX\_TIME | **x** |
| flux | s-1cm-2 | Photon flux of the beamline | NXentry:NXinstrument: NXbeam:flux | NX\_FLOAT:NX\_FLUX | **x** |

**Monochromator**

A monochromator of some sort is used in most of ARPES experiments. The type of monochromator can be inserted in NXentry:NXinstrument:NXmonochromator by using the appropriate sub-elements such as NXgrating, NXmirror, NXfilter, NXcrystal, NXslits.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Name | Unit | Description | Nexus hierarchy | NX variable | NXarpes |
| energy | eV | Central energy | NXentry:NXinstrument:NXmonochromator:energy | NX\_FLOAT:NX\_ENERGY | **v** |
| energy\_error | eV | Energy standard deviation | NXentry:NXinstrument:NXmonochromator:energy\_error | NX\_CHAR | **x** |
| distribution | data | Spectrum or live diagnostic | NXentry:NXinstrument:NXmonochromator:distribution | NXdata | **x** |

Further beam control elements can be implemented using existing NeXus structures, such as NXslits, NXattenuator, NXmirror, etc.

**Manipulator information**

For the manipulator, as generally used in an ARPES experiment, we used the NXpositioner class, that is however used in NeXus documentation only for very raw-level metadata on single motors. We could discuss whether it would be more appropriate to create a NXmanipulator class that directly extends NXinstrument, or to add all the properties to NXsample with the NXtransformation class.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Name | Unit | Description | Nexus hierarchy | NX variable | NXarpes |
| name | None | Name | NXentry:NXinstrument:NXpositioner:name | NX\_CHAR | **x** |
| description | None | Description | NXentry:NXinstrument:NXpositioner:description | NX\_CHAR | **x** |
| type | None | Type of manipulator: “Hexapod”, “Rod”, etc. | NXentry:NXinstrument:NXpositioner:type | NX\_CHAR | **x** |
| pos\_x | um | Position in the x direction | NXentry:NXinstrument:NXpositioner:pos\_x | NX\_FLOAT:NX\_LENGTH | **x** |
| pos\_y | um | Position in the y direction | NXentry:NXinstrument:NXpositioner:pos\_y | NX\_FLOAT:NX\_LENGTH | **x** |
| pos\_z | um | Position in the z direction | NXentry:NXinstrument:NXpositioner:pos\_z | NX\_FLOAT:NX\_LENGTH | **x** |
| pos\_azimuth | deg | Angular position in the azimuthal direction | NXentry:NXinstrument:NXpositioner:pos\_azimuth | NX\_FLOAT:NX\_ANGLE | **x** |
| pos\_tilt | deg | Angular position in the tilt direction | NXentry:NXinstrument:NXpositioner:pos\_tilt | NX\_FLOAT:NX\_ ANGLE | **x** |
| pos\_polar | deg | Angular position in the polar direction | NXentry:NXinstrument:NXpositioner:pos\_polar | NX\_FLOAT:NX\_ ANGLE | **x** |
| cryocoolant | bool | Is cryocoolant flowing through the manipulator? | NXentry:NXinstrument:NXpositioner:pos\_polar | NX\_BOOL | **x** |
| cryostat\_temperature | K | Temperature of the cryostat (coldest point) | NXentry:NXinstrument:NXpositioner:cryostat\_temperature | NX\_FLOAT:NX\_TEMPERATURE | **x** |
| heater\_power | W | Power in the heater for temperature control. | NXentry:NXinstrument:NXpositioner:heater\_power | NX\_FLOAT:NX\_POWER | **x** |
| sample\_temperature | K | Temperature at the closest point to the sample | NXentry:NXinstrument:NXpositioner:sample\_temperature | NX\_FLOAT:NX\_TEMPERATURE | **x** |
| drain\_current | pA | Current to neutralize the photoemission current | NXentry:NXinstrument:NXpositioner:drain\_current | NX\_FLOAT:NX\_CURRENT | **x** |
| sample\_bias | V | Possible bias of the sample with respect to analyser ground | NXentry:NXinstrument:NXpositioner:sample\_bias | NX\_FLOAT:NX\_CURRENT | **x** |

**Detector information**

An analyser is composed of several parts parts: the collection column, the energy dispersion section, the spin dispersion section and the detection section. We would like to open the discussion on whether to further substructure the detector group according to this hierarchy.

**Collection column**

The basic NeXus, conceived for X-ray and Neutrons, is not designed to accommodate the details of electron spectrometers. Most of the matching entries here refer to NXarpes standard.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Name | Unit | Description | Nexus hierarchy | NX variable | NXarpes |
| extractor\_voltage | V | Voltage applied to the extractor lens | NXentry:NXinstrument:NXdetector:extractor\_voltage | NX\_FLOAT:NX\_VOLTAGE | **x** |
| extractor\_current | A | Indicating leakage, field emission or arc currents to the extractor lens | NXentry:NXinstrument:NXdetector:extractor\_current | NX\_FLOAT:NX\_CURRENT | **x** |
| working\_distance | mm | Distance between sample and detector entrance | NXentry:NXinstrument:NXdetector:working\_distance | NX\_FLOAT:NX\_LENGTH | **x** |
| lens\_mode | None | Labelling of a standard lens setting | NXentry:NXinstrument:NXdetector:lens\_mode | NX\_CHAR | **v** |
| lens\_names | None | Set of names of electron optic lenses | NXentry:NXinstrument:NXdetector:lens\_names | NX\_CHAR | **x** |
| lens\_voltages | V | Array of corresponding voltages | NXentry:NXinstrument:NXdetector:lens\_voltages | NX\_FLOAT:NX\_VOLTAGE | **x** |
| projection | None | The space projected in the angularly dispersive directions: “real” or “reciprocal” | NXentry:NXinstrument:NXdetector:projection | NX\_CHAR | **x** |
| magnification | None | The magnification of the projected image in the angularly dispersive direction | NXentry:NXinstrument:NXdetector:magnification | NX\_FLOAT:NX\_DIMENSIONLESS | **x** |
| field\_aperture | um | The size of the field aperture inserted in the column | NXentry:NXinstrument:NXdetector:field\_aperture | NX\_FLOAT:NX\_LENGTH | **x** |
| field\_aperture\_x | mm | Horizontal position of field aperture | NXentry:NXinstrument:NXdetector:field\_aperture\_x | NX\_FLOAT:NX\_LENGTH | **x** |
| field\_aperture\_y | mm | Vertical position of field aperture | NXentry:NXinstrument:NXdetector:field\_aperture\_y | NX\_FLOAT:NX\_LENGTH | **x** |
| contrast aperture | um | Size of contrast aperture inserted in the column | NXentry:NXinstrument:NXdetector:contrast\_aperture | NX\_FLOAT:NX\_LENGTH | **x** |
| contrast\_aperture\_x | mm | Horizontal position of contrast aperture | NXentry:NXinstrument:NXdetector:contrast\_aperture\_x | NX\_FLOAT:NX\_LENGTH | **x** |
| contrast\_aperture\_y | mm | Vertical position of contrast aperture | NXentry:NXinstrument:NXdetector:contrast\_aperture\_y | NX\_FLOAT:NX\_LENGTH | **x** |

**Energy dispersion**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Name | Unit | Description | Nexus hierarchy | NX variable | NXarpes |
| dispersion\_scheme | None | “tof”, “hemispherical”, “cylindrical”, “mirror”, “retarding grid”, etc. | NXentry:NXinstrument:NXdetector:dispersion\_scheme | NX\_CHAR | **x** |
| pass\_energy | eV | Pass energy in dispersive electrodes | NXentry:NXinstrument:NXdetector:pass\_energy | NX\_FLOAT:NX\_ENERGY | **v** |
| center\_energy | eV | Center of the energy window | NXentry:NXinstrument:NXdetector:center\_energy | NX\_FLOAT:NX\_ENERGY | **x** |
| entrance\_slits\_size | um | Size of the entrance slits in dispersive analyzers | NXentry:NXinstrument:NXdetector:entrance\_slit\_size | NX\_FLOAT:NX\_LENGTH | **v** |
| entrance\_slits\_shape | none | “straight” or “curved” | NXentry:NXinstrument:NXdetector:entrance\_slit\_shape | NX\_CHAR | **v** |
| exit\_slits\_size | um | Size of the exit slits in dispersive analyzer | NXentry:NXinstrument:NXdetector:exit\_slit\_size | NX\_FLOAT:NX\_LENGTH | **x** |
| exit\_slits\_shape | None | Shape of the exit slits | NXentry:NXinstrument:NXdetector:exit\_slit\_shape | NX\_CHAR | **x** |
| diameter | mm | Diameter of the dispersive orbit | NXentry:NXinstrument:NXdetector:diameter[[3]](#footnote-3) | NX\_FLOAT:NX\_LENGTH | **x** |
| energy\_scan\_mode | None | “fixed” or “sweep” | NXentry:NXinstrument:NXdetector:acquisition\_mode | NX\_CHAR | **v** |
| tof\_distance | mm | Length of the tof drift electrode | NXentry:NXinstrument:NXdetector:tof\_distance | NX\_FLOAT:NX\_LENGTH | **x** |
| tof\_voltage\* | V | Voltage of the drift electrode | NXentry:NXinstrument:NXdetector:tof\_voltage | NX\_FLOAT:NX\_VOLTAGE | **x** |
| energy\_start | eV | Energy (kinetic) at which the scan starts | NXentry:NXinstrument:NXdetector: energy\_start | NX\_FLOAT:NX\_ENERGY | **x** |
| energy\_step | meV | Energy step of the scan | NXentry:NXinstrument:NXdetector: energy\_step | NX\_FLOAT:NX\_ENERGY | **x** |
| energy\_points | N puro | Total number of energy steps done during the scan | NXentry:NXinstrument:NXdetector: energy\_points | NX\_FLOAT | **x** |
| theta\_x\_start | deg | Angle (along X axis) at which the scan starts | NXentry:NXinstrument:NXdetector:theta\_x\_start | NX\_FLOAT:NX\_ANGLE | **x** |
| theta\_x\_step | deg | Angle (X axis) step of the scan | NXentry:NXinstrument:NXdetector:theta\_x\_step | NX\_FLOAT:NX\_ANGLE | **x** |
| theta\_x\_points | N puro | Total number of angle (X axis) steps done during the scan | NXentry:NXinstrument:NXdetector:theta\_x\_points | NX\_FLOAT | **x** |
| theta\_y\_start | deg | Angle (along Y axis) at which the scan starts | NXentry:NXinstrument:NXdetector:theta\_y\_start | NX\_FLOAT:NX\_ANGLE | **x** |
| theta\_y\_step | deg | Angle (Y axis) step of the scan | NXentry:NXinstrument:NXdetector:theta\_y\_step | NX\_FLOAT:NX\_ANGLE | **x** |
| theta\_y\_points | N puro | Total number of angle (Y axis) steps done during the scan | NXentry:NXinstrument:NXdetector:theta\_y\_points | NX\_FLOAT | **x** |

**Spin dispersion section**

To be discussed and defined. We really put forward only the minimal elements, but we are aware of the variability of spin detectors across the community and hope to hear the opinions of groups that are operating spin resolved instruments on a daily basis.

We added some fields, to be discussed. Note that many are cross linked from the NXsample class and NXdetector energy dispersion section.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Name | Unit | Description | Nexus hierarchy | NX variable | NXarpes |
| spin\_filter\_name | None | Name or model of the spin equipment | NXentry:NXinstrument:name  attribute:@short\_name (acronym) | NX\_CHAR | x |
| spin\_filter\_type | None | Type of spin detector: “VLEED”, “SPLEED”, “Mott”, etc. | NXentry:NXinstrument:NXdetector:spin\_filter\_type | NX\_CHAR | **x** |
| spin\_FoM | None | Figure of merit of the spin detector | NXentry:NXinstrument:NXdetector:spin\_filter\_FoM | NX\_FLOAT | **x** |
| spin\_shermann\_function | None | Effective Shermann function: calibrated spin selectivity factor | NXentry:NXinstrument:NXdetector:spin\_filter\_shermann\_function | NX\_FLOAT | **x** |
| scattering\_chamber | None | “Black” or “White” | NXentry:NXinstrument:NXdetector:scattering\_chamber | NX\_CHAR | **x** |
| spin\_scattering\_energy | eV | Energy of the spin-selective scattering | NXentry:NXinstrument:NXdetector:spin\_scattering\_energy | NX\_FLOAT:NX\_ENERGY | **x** |
| spin\_scattering\_angle | deg | Angle of the spin-selective scattering | NXentry:NXinstrument:NXdetector:spin\_scattering\_angle | NX\_FLOAT:NX\_ANGLE | **x** |
| spin\_target | None | Name of the target | NXentry:NXinstrument:NXdetector:spin\_target | NX\_CHAR | **x** |
| spin\_target\_preparation | None | Preparation procedure of the spin target | NXentry:NXinstrument:NXdetector:spin\_target\_preparation | NX\_CHAR | **x** |
| spin\_target\_preparation\_date | None | Date of last preparation of the spin target | NXentry:NXinstrument:NXdetector:spin\_target\_preparation\_date | NX\_DATETIME | **x** |
| spin\_target\_preparation\_timestamp | s | Unix timestamp | NXentry:NXinstrument:NXdetector:spin\_target\_preparation\_date\_timestamp | NX\_FLOAT | **x** |
| spin\_photon\_energy | eV | The center photon energy at sample | NXentry:NXinstrument:NXsource:photon\_energy | NX\_FLOAT:NX\_ENERGY | **x** |
| spin\_beamline\_slit\_size | um | Beam size along the horizontal direction | Link to the relative info (?) | NX\_FLOAT:NX\_LENGTH | **x** |
| spin\_pass\_energy | eV | Pass energy in dispersive electrodes | NXentry:NXinstrument:NXdetector:pass\_energy | NX\_FLOAT:NX\_ENERGY | **x** |
| spin\_lens\_mode | None | Labelling of a standard lens setting | NXentry:NXinstrument:NXdetector:lens\_mode | NX\_CHAR | **x** |
| spin\_entrance\_slit\_size | um | Size of the entrance slits in dispersive analyzers | NXentry:NXinstrument:NXdetector:entrance\_slit\_size | NX\_FLOAT:NX\_LENGTH | **x** |
| spin\_filter\_slit\_size | None | Size of the entrance slits in the spin detector | NXentry:NXinstrument:NXdetector: spin\_filter\_slit\_size | NX\_FLOAT:NX\_LENGTH | **x** |
| spin\_magnetization\_axis | None | “in plane” or “out of plane” | NXentry:NXinstrument:NXdetector: spin\_magnetization\_axis | NX\_CHAR | **x** |
| spin\_magnetization\_sign | None | “plus” or “minus” | NXentry:NXinstrument:NXdetector: spin\_magnetization\_sign | NX\_CHAR | **x** |
| spin\_sweeps | None | number of sweeps | NXentry:NXinstrument:NXdetector:spin\_sweeps | NX\_FLOAT | **x** |
| spin\_frames | None | number of frames | NXentry:NXinstrument:NXdetector:spin\_frames | NX\_FLOAT | **x** |
| spin\_step\_time | s | Accumulation time spent on each energy step | NXentry:NXinstrument:NXdetector: spin\_step\_time | NX\_FLOAT:NX\_TIME | **x** |
| spin\_energy\_start | eV | Energy (kinetic) at which the scan starts | NXentry:NXinstrument:NXdetector: energy\_start | NX\_FLOAT:NX\_ENERGY | **x** |
| spin\_energy\_step | meV | Energy step of the scan | NXentry:NXinstrument:NXdetector: energy\_step | NX\_FLOAT:NX\_ENERGY | **x** |
| spin\_energy\_points | N puro | Total number of energy steps done during the scan | NXentry:NXinstrument:NXdetector: energy\_points | NX\_FLOAT | **x** |
| spin\_theta\_x\_start | deg | Angle (along X axis) at which the scan starts | NXentry:NXinstrument:NXdetector:theta\_x\_start | NX\_FLOAT:NX\_ANGLE | **x** |
| spin\_theta\_x\_step | deg | Angle (X axis) step of the scan | NXentry:NXinstrument:NXdetector:theta\_x\_step | NX\_FLOAT:NX\_ANGLE | **x** |
| spin\_theta\_x\_points | N puro | Total number of angle (X axis) steps done during the scan | NXentry:NXinstrument:NXdetector:theta\_x\_points | NX\_FLOAT | **x** |
| spin\_theta\_y\_start | deg | Angle (along Y axis) at which the scan starts | NXentry:NXinstrument:NXdetector:theta\_y\_start | NX\_FLOAT:NX\_ANGLE | **x** |
| spin\_theta\_y\_step | deg | Angle (Y axis) step of the scan | NXentry:NXinstrument:NXdetector:theta\_y\_step | NX\_FLOAT:NX\_ANGLE | **x** |
| spin\_theta\_y\_points | N puro | Total number of angle (Y axis) steps done during the scan | NXentry:NXinstrument:NXdetector:theta\_y\_points | NX\_FLOAT | **x** |

**Detection section**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Name | Unit | Description | Nexus hierarchy | NXvariable | NXarpes |
| amplifier\_type | None | Type of electron amplifier: “MCP”, “channeltron”, etc. | NXentry:NXinstrument:NXdetector:amplifier\_type | NX\_CHAR | **x** |
| detector\_type | None | Description of the detector type: “DLD”, “Phosphor+CCD”, “CMOS”. | NXentry:NXinstrument:NXdetector:type | NX\_CHAR | **x** |
| detector\_voltage | V | Voltage applied to detector. | NXentry:NXinstrument:NXdetector:detector\_voltage | NX\_FLOAT:NX\_VOLTAGE | **x** |
| sensor\_size | mm | Size of each imaging sensor chip on the detector. | NXentry:NXinstrument:NXdetector:sensor\_size | NX\_FLOAT:NX\_LENGTH | **x** |
| sensor\_count | Unitless | Number of imaging sensor chips on the detector. | NXentry:NXinstrument:NXdetector:sensor\_count | NX\_INT:NX\_UNITLESS | **x** |
| sensor\_pixel\_size | um | Physical size of the pixels of the imaging chip on the detector. | NXentry:NXinstrument:NXdetector:x\_pixel\_size  NXentry:NXinstrument:NXdetector:y\_pixel\_size | NX\_FLOAT:NX\_LENGTH | **x** |

**Sample information**

More options are available in the NeXus hierarchy that may be less related to ARPES samples.

Note that the temperature is cross linked from the sample\_temperature field in the manipulator, as an example of cross linking data from NXinstrument hierarchy in more elevated and descriptive hierarchy positions.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Name | Unit | Description | Nexus hierarchy | NXvariable | NXarpes |
| name | None | Simple and descriptive name of the sample | NXentry:NXsample:name | NX\_CHAR | **v** |
| sample\_id | None | Identification number or signatures of the sample used. | NXentry:NXsample:sample\_id | NX\_CHAR | **x** |
| state | None | Physical state of the sample[[4]](#footnote-4) | NXentry:NXsample: state | NX\_CHAR | **x** |
| purity | None | Chemical purity of the sample | NXentry:NXsample: purity | NX\_FLOAT:NX\_UNITLESS | **x** |
| surface\_orientation | None | Surface termination of the sample (if crystalline) | NXentry:NXsample: surface\_orientation | NX\_CHAR | **x** |
| layer | None | Number of layers of the sample (e.g. “bulk”, “monolayer”, “pentalayer”, etc.) | NXentry:NXsample: layer | NX\_CHAR | **x** |
| sample\_space\_group | None | Space group of the sample (if crystalline) | NXentry:NXsample: space\_group | NX\_CHAR | **x** |
| chemical\_formula | None | Chemical formula of the sample | NXentry:NXsample: chemical\_formula | NX\_CHAR | **x** |
| chemical\_name | None | Full chemical name of the sample | NXentry:NXsample: chemical\_name | NX\_CHAR | **x** |
| chem\_id\_cas | None | CAS registry number of the sample’s chemical content. | NXentry:NXsample: chem\_id\_cas | NX\_CHAR | **x** |
| temperature | K | Temperature of the sample during the measurement. | NXentry:NXinstrument:NXpositioner:sample\_temperature | NX\_FLOAT:NX\_TEMPERATURE | **x** |
| drain\_current | pA | Current to neutralize the photoemission current | NXentry:NXinstrument:NXpositioner:drain\_current | NX\_FLOAT:NX\_CURRENT | **x** |
| sample\_bias | V | Possible bias of the sample with respect to analyser ground | NXentry:NXinstrument:NXpositioner:sample\_bias | NX\_FLOAT:NX\_CURRENT | **x** |
| pressure | Pa | Pressure of gas surrounding the sample at time of measurement. | NXentry:NXsample: pressure | NX\_FLOAT:NX\_PRESSURE | **x** |
| gas | None | Gases might be fluxed on the surface for various reasons. Chemical designation, or “residual”. | NXentry:NXsample: gas | NX\_CHAR | **x** |
| E\_field | V | Electric field applied across the sample. Different from sample\_bias. | NXentry:NXsample:electric\_field  @direction | NX\_FLOAT:NX\_VOLTAGE | **x** |
| B\_field | T | Magnetic field applied to the sample during the measurement. | NXentry:NXsample:emagnetic\_field  @direction | NX\_FLOAT:NX\_ANY | **x** |
| stress\_field | Pa | Stress field applied to the sample during the measurement. | NXentry:NXsample:stress\_field  @direction | NX\_FLOAT:NX\_PRESSURE | **x** |
| thickness | mm | Sample thickness | NXentry:NXsample:thickness | NX\_FLOAT:NX\_LENGTH | **x** |
| surface\_dopant | None | Element of evaporated surface dopant such as alkali or other | NXentry:NXsample:surface\_dopant | NX\_CHAR | **x** |
| surface\_dopant\_coverage | Å | Nominal thickness of the evaporated dopant | NXentry:NXsample:surface\_dopant\_coverage | NX\_FLOAT:NX\_LENGTH | **x** |
| bias\* | V | Voltage applied to sample and sample holder. | NXentry:NXsample:bias | NX\_CHAR | **x** |
| drain\_current | A | Drain current due to photoemission | NXentry:NXsample:drain\_current | NX\_FLOAT:NX\_CURRENT | **x** |
| growth\_method | None | Sample growth method (e. g. molecular beam epitaxy, chemical vapor deposition etc.) | NXentry:NXsample:growth\_method | NX\_FLOAT:NX\_CURRENT | **x** |
| preparation\_method | None | E.g. “UHV cleave”, “sputtering and annealing”, etc. | NXentry:NXsample:preparation\_method | NX\_FLOAT:NX\_CURRENT | **x** |
| preparation\_date | Date | Date of sample preparation | NXentry:NXsample:preparation\_date | NX\_DATE\_TIME | **x** |
| preparation\_date\_timestamp | s | UNIX timestamp of sample preparation | NXentry:NXsample:preparation\_date\_timestamp | NX\_FLOAT:NX\_TIME | **x** |
| vendor | None | Name of the sample vendor (company or research group) | NXentry:NXsample:vendor | NX\_CHAR | **x** |
| substrate\_material | None | Material of the substrate in direct contact with the sample. | NXentry:NXsample:substrate\_material | NX\_CHAR | **x** |
| substrate\_state | None | Physical state of the substrate, similar options to sample\_state | NXentry:NXsample:substrate\_state | NX\_CHAR | **x** |
| substrate\_vendor | None | Vendor of the substrate material | NXentry:NXsample:substrate\_material | NX\_CHAR | **x** |
| sample\_notes | None | Further notes. | NXentry:NXsample:notes | NX\_CHAR | **x** |

**Processing Information**

NeXus has a NXprocess base class, that however is not further structured. We are interested in expanding this, with a full hierarchy for complex preprocessing. For this we had to create new NXclasses that extend NXprocess: NXdistortion, NXregistration, NXcorrection, NXenhancement.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Name | Unit | Description | Nexus hierarchy | NX variable | NXarpes |
| program\_name | None | Name of the processing program or script | NXentry:NXprocess:program | NX\_CHAR | **x** |
| program\_version | None | Version of the program or script | NXentry:NXprocess: version | NX\_CHAR | **x** |
| program\_codebase | None | Set of libraries/tools used in the program/script | NXentry:NXprocess:program\_codebase | NX\_CHAR | **x** |
| program\_sequence | None | Sequence of transformations applied to the data, as some are non-commutative | NXentry:NXprocess:program\_sequence | NX\_CHAR | **x** |
| calculated\_kx | Å-1 | calibrated kx momentum axis | NXentry:NXprocess:calculated\_kx | NX\_FLOAT:NX\_WAVENUMBER | **x** |
| calculated\_ky | Å-1 | calibrated ky momentum axis | NXentry:NXprocess:calculated\_ky | NX\_FLOAT:NX\_WAVENUMBER | **x** |
| calculated\_energy | eV | Calibrated energy axis | NXentry:NXprocess:calculated\_energy | NX\_FLOAT:NX\_ENERGY | **x** |
| calculated\_delay | fs | Calibrated Delay stage position | NXentry:NXprocess:calculated\_delay | NX\_FLOAT:NX\_TIME | **x** |
| calculated\_x\_to\_kx | Å-1 | Pixel x axis to kx momentum calibration | NXentry:NXprocess:calculated\_x\_to\_kx | NX\_DATA | **x** |
| calculated\_y\_to\_ky | Å-1 | Pixel y axis to ky momentum calibration | NXentry:NXprocess:calculated\_x\_to\_ky | NX\_DATA | **x** |
| calculated\_tof\_to\_energy | eV | Time\_of\_flight to energy calibration | NXentry:NXprocess:calculated\_tof\_to\_energy | NX\_DATA | **x** |
| calculated\_stage\_to\_delay | fs | Delay stage calibration | NXentry:NXprocess:calculated\_stage\_to\_delay | NX\_DATA | **x** |
| other\_converts | None | Conversion factors between other measured and physical axes. | NXentry:NXinstrument:NXdetector:other\_converts | NX\_DATA | **x** |
| theta\_x\_vect |  |  | NXentry:NXprocess: theta\_x\_vect | NX\_DATA | **x** |
| theta\_y\_vect |  |  | NXentry:NXprocess: theta\_y\_vect | NX\_DATA | **x** |
| kinetic\_energy\_vect |  |  | NXentry:NXprocess: kinetic\_energy\_vect | NX\_DATA | **x** |

**Distortion correction**

We propose the class **NXdistortion**. Our perspective on symmetry based distortion correction is in [Xian et al.](https://doi.org/10.1016/j.ultramic.2019.04.004) These parameters are based on our experience, but meant to be expanded to meet the different procedures in the whole community.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Name | Unit | Description | Nexus hierarchy | NX variable | NXarpes |
| applied | Bool | Has the distortion correction been applied? | NXentry:NXprocess:NXdistortion:applied | NX\_BOOL | **x** |
| symmetry | None | Number of elementary symmetry operations. | NXentry:NXprocess:NXdistortion:symmetry | NX\_INT | **x** |
| symmetry\_angle | deg | Degrees of rotation for a symmetry operation. | NXentry:NXprocess:NXdistortion:symmetry\_angle | NX\_FLOAT:NX\_INT | **x** |
| original\_centre | None | Coordinates of the symmetry centre point. | NXentry:NXprocess:NXdistortion:original\_centre | NX\_FLOAT | **x** |
| original\_points | None | Coordinates of the relevant symmetry points. | NXentry:NXprocess:NXdistortion:original\_points | NX\_FLOAT | **x** |
| Field | None | 2D matrix mapping the original distorted field in the undistorted one. | NXentry:NXprocess:NXdistortion:field | NX\_FLOAT | **x** |

**Image registration**

Rigid translation and rotation of the image. We propose the class **NXregistration**.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Name | Unit | Description | Nexus hierarchy | NX variable | NXarpes |
| applied | Bool | Has the registration been applied? | NXentry:NXprocess:NXregistration:applied | NX\_BOOL | **x** |
| x\_translation | None | Horizontal translation | NXentry:NXprocess:NXregistration:x\_translation | NX\_FLOAT | **x** |
| y\_translation | None | Vertical translation | NXentry:NXprocess:NXregistration:y\_translation | NX\_FLOAT | **x** |
| new\_centre | None | Coordinates of the new symmetry centre point. | NXentry:NXprocess:NXregistration:new\_centre | NX\_FLOAT | **x** |
| rotation\_centre | None | Coordinates of the rotation centre. | NXentry:NXprocess:NXregistration:rotation\_centre | NX\_FLOAT | **x** |
| rotation\_angle | Deg | Angle of rotation | NXentry:NXprocess:NXregistration:rotation\_angle | NX\_FLOAT:NX\_ANGLE | **x** |
| scaling | None | Scaling factor to compensate shrinking from distortion correction. | NXentry:NXprocess:NXregistration:scaling | NX\_FLOAT | **x** |

**Image calibration**

Energy and momentum calibration parameters are grouped in the **NXcalibration** class. To be expanded and perfected. Further parameters may be needed depending on the specifics of the data treatment.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Name | Unit | Description | Nexus hierarchy | NX variable | NXarpes |
| applied | Bool | Has the calibration been applied? | NXentry:NXprocess:NXcalibration:applied | NX\_BOOL | **x** |
| coefficients | None | Array of coefficients of the calibration function for non linear calibration | NXentry:NXprocess:NXcalibration:coefficients | NX\_FLOAT | **x** |
| features | Not specified | Array of position of features along the axis to be calibrated | NXentry:NXprocess:NXcalibration:features | NX\_FLOAT | **x** |
| destinations | Not specified | Array of destinations in the calibrated axis | NXentry:NXprocess:NXcalibration:destinations | NX\_FLOAT | **x** |
| files | None | Files used for the calibration | NXentry:NXprocess:NXcalibration:files | NX\_CHAR | **x** |
| scaling | Not specified | Scaling parameter for linear calibration | NXentry:NXprocess:NXcalibration:scaling | NX\_FLOAT | **x** |
| offset | Not specified | Offset parameter for linear calibration | NXentry:NXprocess:NXcalibration:offset | NX\_FLOAT | **x** |

**Data**

The data inserted as the multidimensional volume in expected in the standard NXentry:NXdata class, with @signal attribute. The axes can be any suitably dimensioned array in the entry, referred to in the NXdata object with the @axes attribute. The do not need to be repeated in the creation of the NXdata group, they can simply be linked.

In our case, for example, the axes are linked from NXentry:NXprocess:calculated\_kx, NXentry:NXprocess:calculated\_ky, NXentry:NXprocess:calculated\_energy and NXentry:NXprocess:calculated\_delay. See the examples for further clarification.

In APE case, the axes are linked from NXentry:NXprocess:theta\_x\_vect, NXentry:NXprocess:theta\_y\_vect, NXentry:NXprocess:kinetic\_energy\_vect

1. Possible values (photoemission): Synchrotron X-ray Source, Rotating Anode X-ray, Fixed Tube X-ray, UV Laser, Free-Electron Laser, Optical Laser, UV Plasma Source. [↑](#footnote-ref-1)
2. Possible values (photoemission): x-ray, ultraviolet, visible light. [↑](#footnote-ref-2)
3. Designed for cylindrical particle detectors, but in this case, the hierarchy is not confusing and this group can be recycled. [↑](#footnote-ref-3)
4. Should be one of the following “gas”, “liquid”, “solution”, “amorphous solid”, “vitreous solid”, “monocrystalline solid”, “polycrystalline solid”, “plasma”, “dark matter”, “negative mass matter”, “strange matter”, “onium”, “quark-gluon plasma”, “BEC”, “FDC”, “nuclear pasta”, “tachyon condensate”, “photonic matter”, etc. As an Italian, I am particularly intrigued by nuclear pasta. [↑](#footnote-ref-4)