XAS Detection Modes

The goal of this file is to document in a simpler collaborative way the **"mode" mandatory field of the NXxas class**. The "mode" will be defined as "NXxas_mode" class, consisting in a list of possible choices, with eventually additional mandatory fields. The "mode" is there to unequivocally define what is given for the "intensity" array of NXxas. Furthermore, in the description of each mode we need to specify what additional information is mandatory and what is recommended.

For the sake of clarity, the current **minimum mandatory entries** in NXxas are:

- energy
- intensity
- mode
- element → NXelement (new)
- edge → NXedge (new)
- sample / name → NXsample (https://manual.nexusformat.org/classes/base_classes/NXsample.html)

Some examples of converted files to NXxas are given at https://pynxxas.readthedocs.io/en/latest/

Once this document is finished, it will be translated to the nxdl language into https://github.com/XraySpectroscopy/nexus_definitions and then submitted to the NIAC for approval.

The current build of the definition documentation is available at

https://hdf5.gitlab-pages.esrf.fr/nexus/nxxas/classes/applications/NXxas_new.html

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NXxas_mode

NOTE (common to all modes): **the "intensity" array should represent a normalized XAS-like spectrum**, that is, a step-like shape with values ranging around 0-1. Furthermore, it is recommended to provide the raw measured data and the processing steps or metadata necessary to obtain such an array.

1. **Transmission**

   Direct measurement of the absorption coefficient $\mu(E) = -\ ln(Itrans/I0)$ by measuring the beam intensity before (I_0) and after the sample (I_{trans}). The details of how I_0/I_{trans} are measured should go as NXinstrument

(https://manual.nexusformat.org/classes/base_classes/NXinstrument.html#nxinstrument)

"intensity" is -ln(I_{trans}/I_0)

<u>recommended:</u>

- I_{trans}: intensity transmitted beam
- I_0: incoming beam intensity

2. **Partial fluorescence yield (PFY)**

Partial fluorescence yield uses an energy-dispersive detector - like a Silicon-drift diode or High-Purity Ge detector (one or multiple channels) - to select a portion of the fluorescence and scattered signal. Typically only energies around a selected fluorescence line of the absorbing element are selected, such as Kalpha, rejecting all other energies. A region of interest (ROI) of the multi-channel analyzer (MCA) spectrum is given for the fluorescence signal - summed over multiple channels (I_f). The given I_f should be corrected by dead-time. In this mode $\mu(E) \propto I_f/I_0$ and may be affected by self-absorption effects that should be corrected, whatever possible.

"intensity" is I_f/I_0

<u>recommended:</u>

- I_0: incoming beam intensity
- I_f: for each channel (i) of the detector
- emission line(s) in the ROI
- $MCA(E)_i$: multi-channel analyzer spectrum for each energy
- dead-time correction constant or livetime information
- applied self-absorption correction, if any

3. **Total fluorescence yield (TFY)**

This is the case where the total fluorescence signal is measured with a fluorescence detector, like a photodiode.

"intensity" is I_f/I_0

<u>recommended:</u>

- I_0: incoming beam intensity
- I_f: for each channel (i) of the detector

3. **High-energy resolution fluorescence detection (HERFD)**

Particular case of partial fluorescence yield measured with a crystal analyzer spectrometer with an energy bandwidth around 1-2 eV. In this case what is measured is a diagonal cut of a Resonant Inelastic X-ray Scattering (RIXS) plane. The obtained XAS-like spectrum strongly depends on the emission energy where it is measured, thus this information is mandatory.

"intensity" is I_f/I_0

mandatory:

- emission line → NXemission_lines
- emission energy

recommended:

- I_0
- I_f
- energy bandwidth or resolution of the spectrometer
- energy bandwidth or resolution of incoming beam monochromator

4. **Wavelength-Dispersive and Transition Edge Sensor (TES)**

   Particular case for fluorescence-detection with an experimental setup that gives an energy resolution that is in between PFY and HERFD, usually in the order of 10-20 eV.

   "intensity" is I_f/I_0

   recommended:

   - I_0
   - I_f
   - emission line
   - emission energy
   - energy bandwidth or resolution of the spectrometer
   - energy bandwidth or resolution of incoming beam monochromator

5. **Electron yield (EY)**

   Here the XAS spectrum is measured via the collection of the secondary Auger electrons. Measuring the intensity of electrons emitted from the sample is electron yield (I_{EY}), which can either be Total (TEY) - measuring all electrons, Partial (PEY) - applying a voltage gradient to select an energy range or Conversion (CEY) - using a gas to create conversion electrons. Electrons are readily absorbed by most materials so this technique is surface sensitive.

“intensity” is I_{EY}/I_0

<u>recommended:</u>

- I_0
- I_{EY}
- type: TEY, PEY, CEY

6. **Energy Dispersive (ED)**

This mode measures a polychromatic incoming beam I_0 and the transmitted beam is energy-dispersed/analyzed by a polychromator I_{trans}

“intensity” is I_{trans}/I_0

<u>recommended</u>

- I_0
- I_{trans}
- polychromator energy resolution/bandwidth

7. **X-ray Raman Scattering (XRS)**

“intensity” is the I_0-normalized contribution to the double-differential cross section S(q,w) from the shell of interest, extracted from the total nonresonant IXS signal by subtracting the Compton background.

<u>mandatory</u>

- q vector

<u>recommended</u>

- I_0
- raw intensity of the nonresonant IXS signal
- how the Compton background is subtracted

8. Diffraction Anomalous Fine Structure (DAFS)

The intensity of a diffraction peak is monitored as a function of incoming monochromatic X-rays. The signal should be reported as f″(E). It is recommended to provide as RAW_DATA the measured intensity and describe the steps used to extract the signal.

9. Electron energy loss (EELS)

10. Inverse partial fluorescence yield (IPFY)

If the absorption by the element of interest is strong, then monitoring the scattered intensity away from the fluorescence can be used to monitor what is absorbed by the

11. X-ray Excited Optical Luminescence (XEOL)
    Partial optical yield measured as function of the incoming monochromatic X-rays
12. Total reflection Extended X-ray Absorption Fine Structure (ReflEXAFS)
    In this mode the reflectivity signal is measured. The signal should be reported as f″(E). It is recommended to provide as RAW_DATA the measured reflectivity and describe the steps used to extract the signal.
13. Grazing Incidence X-ray Fluorescence (GIXRF)
    The fluorescence yield is measured at grazing incidence angle
14. Grazing Emission X-ray Fluorescence (GEXRF)
    The fluorescence yield is measured at grazing emission angle

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NXxas schema (probably separate document):

NXxas:
  definition string, NeXuS class name == "NXxas"
  absorption_edge string, absorption edge, 'K', L3', ...
  element string, element symbol, 'S', 'Fe', ...
  mode string, name of measurement mode, 'Transmission', 'Fluorescence', ...
  title string, description of spectrum
  energy array, energy values
    attributes: 'units' 'eV', 'keV'
  intensity array, absorption values: pre-edge subtracted, normalized mu(E)
  reference string, name of group to use for energy reference
  instrument NXGroup describing instruments used for measurements
  scan NXGroup describing data collection, if available.
  plot NXGroup for "easily plottable data"
  process NXGroup for description of conversion of rawdata to normalized mu(E) intensity.
  rawdata Dataset containing N-dmensional array (Narrays, Nenergy) of "as collected" data used to generate "intensity".
    attributes: 'array_labels' labels for Narray columns

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  instrument:

beamline NXGroup with information about "beamline" used and X-ray optics conditions
source NXGroup with information about X-ray source used.
monochromator NXGroup with information about X-ray monochromator used.
i0 NXGroup with information about detector used for I0
itrans NXGroup with information about detector used for Transmission (if used)
ifluor NXGroup with information about detector used for Fluorescence or Emission (if used)

scan:
edge_energy string, edge energy used
comments string, description of data collection
headers string, headers from raw data file, if available
start_time string, date and time of scan

plot:
energy link to top-level "energy"
intensity link to top-level "intensity"

process:
date string, date and time processed
notes string, description, perhaps code of processing done and values used to convert "rawdata" group to "intensity" array.
program string, name of program used
version string, version of program used

Notes:

1. Instrument/monochromator NXGroup has
   instrument/monochromator/crystal/d_spacing d-spacing used (may be a string or float)
   instrument/monochromator/crystal/type crystal used (for example, "Si")
   instrument/monochromator/crystal/reflection array of reflection (for example, [1, 1, 1])
2. Instrument Detector Groups can have any name (i0, itrans, etc) and will have structure like:
   instrument/i0/data Array of I0 data
   instrument/i0/description String describing detector
3. Instrument/beamline and Instrument/source both contain sets of strings for describing beamline and source.
4. Multiple "rawdata" groups can be used -- use any name for an HDF5 Dataset, and reference that in the "process" group.
5. the "plot" Group is common in NeXuS, meant for tools to always be able to find a simple way to display data.

Notes from meeting:

add monochromator comments
add Sample
add Relevant Fields that might make use of the spectrum.