Extracted from FeXas.nxs attached to e-mail from Abraham.

FeFoil.001 is the entry name;

Smr notes added

Variable names – ddi/cdi variables…

Serialization scheme

# FeFoil.001/ (Group)

attributes:

## FeFoil.001/data/ (Group) [this group provides two arrays for presenting a plot of the observed data; as a variable suggest this should be something like ‘dataForPlotting’]

attributes: none

### FeFoil.001/data/mode (Dataset); [enumeration: { "Total Electron Yield" ,"Partial Electron Yield","Auger Electron Yield","Fluorescence Yield","Transmission"}]

shape: (), dims: 0; dtype: object

**Data value: Transmission**

### FeFoil.001/data/mufluor (Dataset); [mu is typically the linear attenuation coefficient (µ), which quantifies the overall reduction in the intensity of a narrow beam of X-rays per unit thickness of the material. It accounts for both absorption and scattering. The units for µ are typically inverse length units like cm⁻¹. not clear what mufluor and mutrans are; NXML for NXxas has data/absorbed\_beam and data/energy in NXData (i.e. entry/data or in this case FeFoil.001/data)]

shape: (443,), dims: 1; dtype: float64

### FeFoil.001/data/mutrans (Dataset);

shape: (443,), dims: 1; dtype: float64

## FeFoil.001/definition (Dataset);

shape: (), dims: 0; dtype: object

Data value: Nxxas[this is the application profile]

attributes: none

## FeFoil.001/start\_time (Dataset); [discovery metadata]

shape: (), dims: 0; dtype: object

Data value: 2020-08-10 09:18:48

attributes: none

## FeFoil.001/title (Dataset); [discovery metadata]

shape: (), dims: 0; dtype: object

Data value: FeFoil.001 [Fe K edge]

## FeFoil.001/instrument/ (Group)

attributes: none

### FeFoil.001/instrument/i0/ (Group)

attributes: none [units--???counts??]

FeFoil.001/instrument/i0/data (Dataset); [incident intensity?]

shape: (443,), dims: 1; dtype: float64

### FeFoil.001/instrument/ifluor/ (Group)

attributes: none

#### FeFoil.001/instrument/ifluor/data (Dataset); [observed flourescence intensity????]

shape: (443,), dims: 1; dtype: float64

#### FeFoil.001/instrument/ifluor/mode (Dataset); [????]

shape: (), dims: 0; dtype: object

Data value: Unknown

### FeFoil.001/instrument/itrans/ (Group)

attributes: none

#### FeFoil.001/instrument/itrans/data (Dataset); [observed transmitted intensity]

shape: (443,), dims: 1; dtype: float64

### FeFoil.001/instrument/monochromator/ (Group)

attributes: none

#### FeFoil.001/instrument/monochromator/crystal/ (Group)

attributes: none

##### FeFoil.001/instrument/monochromator/crystal/chemical\_formula [configuration] (Dataset); [in xdi header, but those also have crystal face e.g.’S’i 111’]

shape: (), dims: 0; dtype: object

Data value: Si

##### FeFoil.001/instrument/monochromator/crystal/d\_spacing (Dataset); [in xdi header, leave in HDF file? Should this be listed as a variable? Not in NXML NXxas application]

shape: (), dims: 0; dtype: float64

attributes: none

##### FeFoil.001/instrument/monochromator/crystal/reflection (Dataset); [details, leave in HDF file? Should this be listed as a variable? Not in NXML NXxas application]

shape: (3,), dims: 1; dtype: int64

#### FeFoil.001/instrument/monochromator/energy (Dataset);

shape: (443,), dims: 1; dtype: float64

attributes: units (eV)

### FeFoil.001/instrument/source/ (Group)

attributes: none

#### FeFoil.001/instrument/source/name (Dataset); [discovery metadata]

shape: (), dims: 0; dtype: object

Data value: APS, undulator 36mm, 66 poles, 13-ID-E [discovery metadata]

#### FeFoil.001/instrument/source/probe (Dataset);

shape: (), dims: 0; dtype: object

Data value: X-ray

#### FeFoil.001/instrument/source/type (Dataset); [discovery metadata]

shape: (), dims: 0; dtype: object

Data value: X-ray Source [isn’t there some more specific way to identify the kind of source?]

[the rest of these are not in the NXxas application spec; should any of these be exposed in the metadata?]

#### FeFoil.001/ instrument/source/energy (Dataset); [? Discovery metadata?]

shape: (), dims: 0; dtype: float64

attributes: none

#### FeFoil.001/ instrument/source/facility\_energy (Dataset); [this in in the XDI header]

shape: (), dims: 0; dtype: object

Data value: 7.0 GeV

#### FeFoil.001/ instrument/source/facility\_name (Dataset); [this in in the XDI header]

shape: (), dims: 0; dtype: object

Data value: APS

#### FeFoil.001/ instrument/source/facility\_ring\_current (Dataset); [this in in the XDI header ‘facility.current’?]

shape: (), dims: 0; dtype: object

Data value: 101.9

#### FeFoil.001/ instrumentsource/facility\_xray\_source (Dataset); [this in in the XDI header]]

shape: (), dims: 0; dtype: object

Data value: undulator 36mm, 66 poles

#### FeFoil.001/instrument/source/beamline\_name (Dataset); [this in in the XDI header]

shape: (), dims: 0; dtype: object

Data value: 13-ID-E

#### FeFoil.001/instrument/source/beamline\_harmonic\_rejection (Dataset); [this in in the XDI header]

shape: (), dims: 0; dtype: object

Data value: 2 Si mirrors, 3 mrad

#### FeFoil.001/instrument/source/beamline\_fluxestimate (Dataset);

shape: (), dims: 0; dtype: object

Data value: 6.57399e+09

#### FeFoil.001/instrument/source/beamline\_foe\_slit\_hpos (Dataset);

shape: (), dims: 0; dtype: object

Data value: 0

#### FeFoil.001/instrument/source/beamline\_foe\_slit\_hwid (Dataset);

shape: (), dims: 0; dtype: object

Data value: 0.4000

#### FeFoil.001/instrument/source/beamline\_foe\_slit\_vpos (Dataset);

shape: (), dims: 0; dtype: object

Data value: 0

#### FeFoil.001/instrument/source/beamline\_foe\_slit\_vwid (Dataset);

shape: (), dims: 0; dtype: object

Data value: 0.2000

#### FeFoil.001/instrument/source/beamline\_i0\_sensitivity\_number (Dataset);

shape: (), dims: 0; dtype: object

Data value: 50

#### FeFoil.001/instrument/source/beamline\_i0\_sensitivity\_unit (Dataset);

shape: (), dims: 0; dtype: object

Data value: pA/V

#### FeFoil.001/instrument/source/beamline\_i0volts2fluxout (Dataset);

shape: (), dims: 0; dtype: object

Data value: 3.00892e+09

#### FeFoil.001/instrument/source/beamline\_i1\_sensitivity\_number (Dataset);

shape: (), dims: 0; dtype: object

Data value: 100

#### FeFoil.001/instrument/source/beamline\_i1\_sensitivity\_unit (Dataset);

shape: (), dims: 0; dtype: object

Data value: pA/V

#### FeFoil.001/instrument/source/beamline\_i2\_sensitivity\_number (Dataset);

shape: (), dims: 0; dtype: object

Data value: 20

#### FeFoil.001/instrument/source/beamline\_ssa\_slit\_hpos (Dataset);

shape: (), dims: 0; dtype: object

Data value: 0

#### FeFoil.001/instrument/source/beamline\_ssa\_slit\_hwid (Dataset);

shape: (), dims: 0; dtype: object

Data value: 0.0150

#### FeFoil.001/instrument/source/beamline\_ssa\_slit\_vpos (Dataset);

shape: (), dims: 0; dtype: object

Data value: 0.4500

#### FeFoil.001/instrument/source/beamline\_ssa\_slit\_vwid (Dataset);

shape: (), dims: 0; dtype: object

Data value: 0.5000

#### FeFoil.001/instrument/source/facility\_ring\_lifetime (Dataset);

shape: (), dims: 0; dtype: object

Data value: 9.0

## FeFoil.001/sample/ (Group) [shouldn’t there be explicit information about what was analyzed?]

attributes: none

**missing** sample/name

## FeFoil.001/scan/ (Group) [not in NXML NXxas application definition, looks like NXscan class; this is probably raw data???]

attributes: none

### FeFoil.001/scan/column\_labels (Dataset);

shape: (35,), dims: 1; dtype: object

### FeFoil.001/scan/data (Dataset);

shape: (443, 35), dims: 2; dtype: float64

### FeFoil.001/scan/edge\_energy (Dataset);

shape: (), dims: 0; dtype: object

Data value: 7112.000

### FeFoil.001/scan/end\_time (Dataset);

shape: (), dims: 0; dtype: object

Data value: 2020-08-10 09:22:32

### FeFoil.001/scan/legend (Dataset);

shape: (), dims: 0; dtype: object

Data value: Start, Stop, Step, K-space, Time

### FeFoil.001/scan/nCol (Dataset);

shape: (), dims: 0; dtype: int64

### FeFoil.001/scan/nP (Dataset);

shape: (), dims: 0; dtype: int64

### FeFoil.001/scan/region1 (Dataset);

shape: (), dims: 0; dtype: object

Data value: -60.000, -10.000, 2.500 False 0.50

### FeFoil.001/scan/region2 (Dataset);

shape: (), dims: 0; dtype: object

Data value: -10.000, 19.997, 0.100 False 0.50

### FeFoil.001/scan/region3 (Dataset);

shape: (), dims: 0; dtype: object

Data value: 2.291, 8.500, 0.050 True 0.50

### FeFoil.001/scan/scan\_mode (Dataset);

shape: (), dims: 0; dtype: object

Data value: Unknown

### FeFoil.001/scan/start\_time (Dataset); [same as FeFoil.001/start\_time]

shape: (), dims: 0; dtype: object

Data value: 2020-08-10 09:18:48

### FeFoil.001/scan/xrayedge/ (Group)

attributes: none

#### FeFoil.001/scan/xrayedge/edge (Dataset);

shape: (), dims: 0; dtype: object

Data value: K

#### FeFoil.001/scan/xrayedge/element (Dataset);

shape: (), dims: 0; dtype: object

Data value: Fe