SciCat at P08

overview

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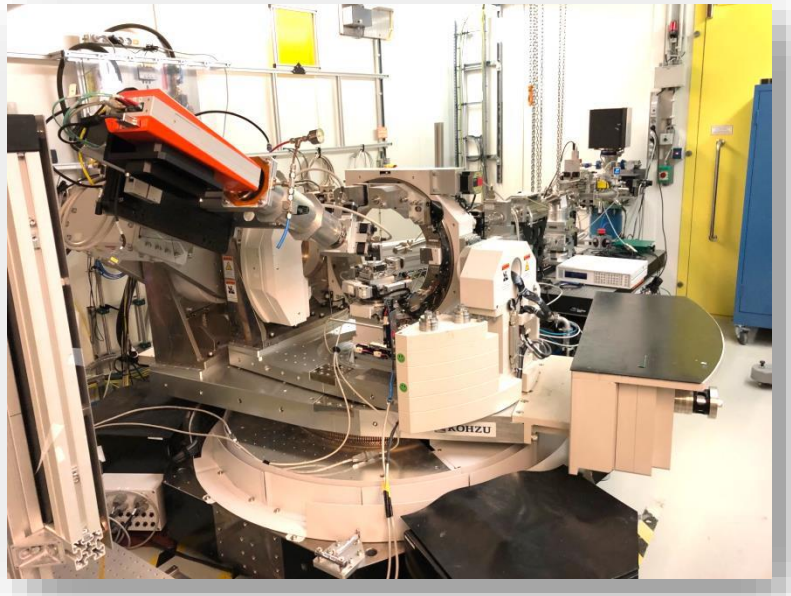
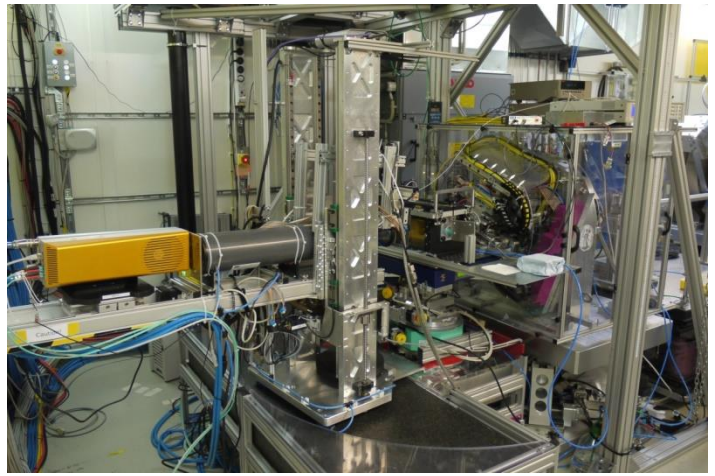
DESY

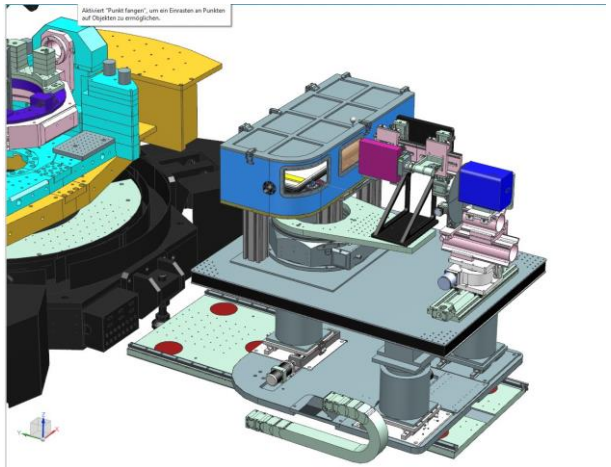
Experimental Setups



6 circle diffractometer (P08)



Liquid diffractometer (P08)



Langmuir GID setup (P08)

Science case:

X-ray diffraction and scattering experiments mostly on thin films, surfaces, interfaces and nanostructures

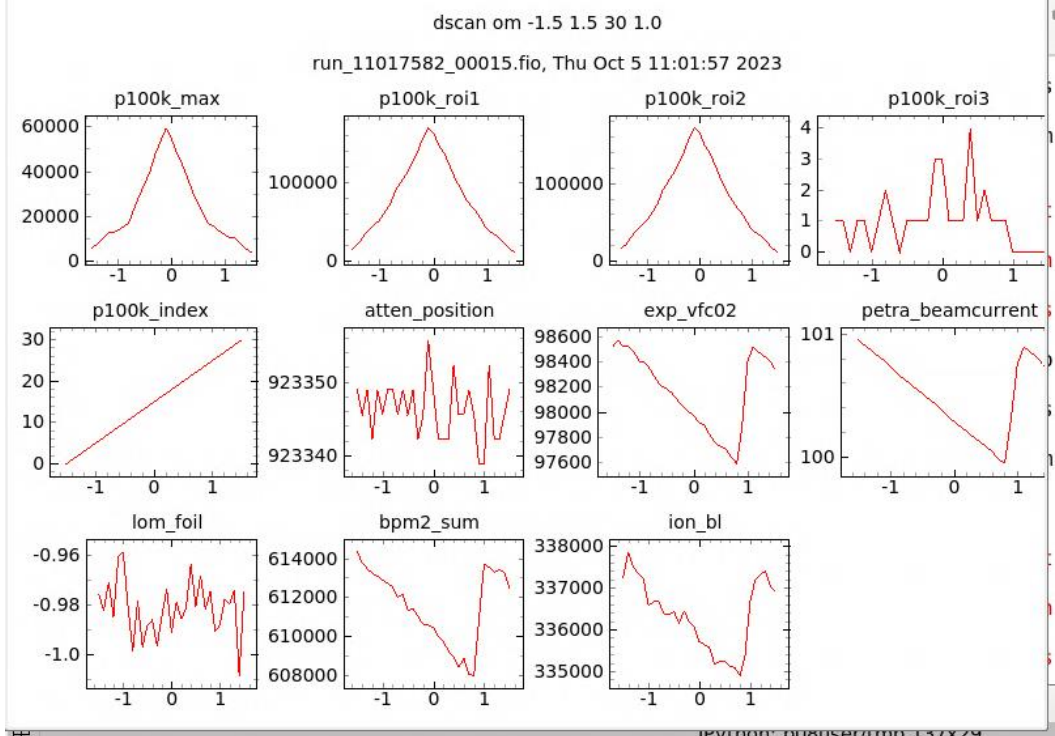
Data acquisition & representation

Typical measurement:

- step-wise motion of one or more rotations recording one image at each position (typical framerate: 0.1-10Hz)
- time resolved measurements at fixed position (typical framerate: 0.1-10Hz; sometimes 1kHz for short time, e.g. 10s)

Usually we use 2D detectors but represent them by summing user defined regions of interest (roi) for simpler representation of the scan data.

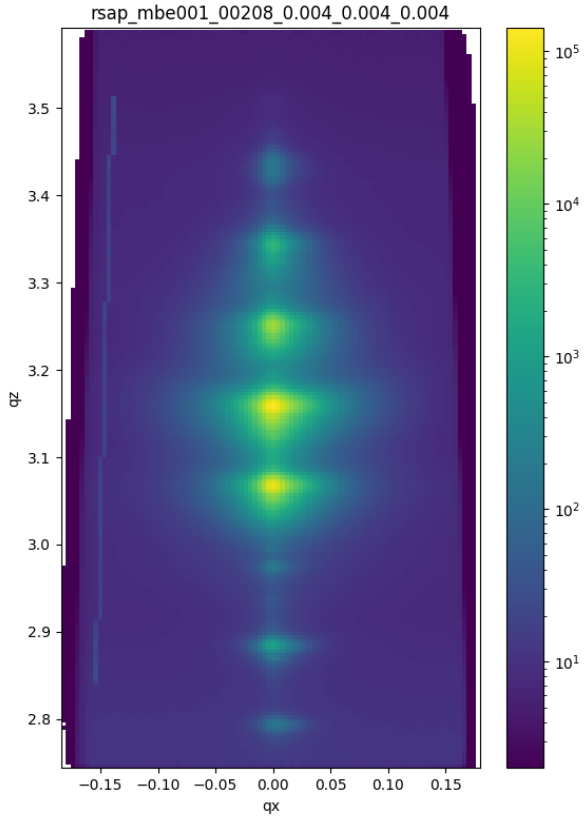
Here the scan is added to the list of files to be ingested into SciCat



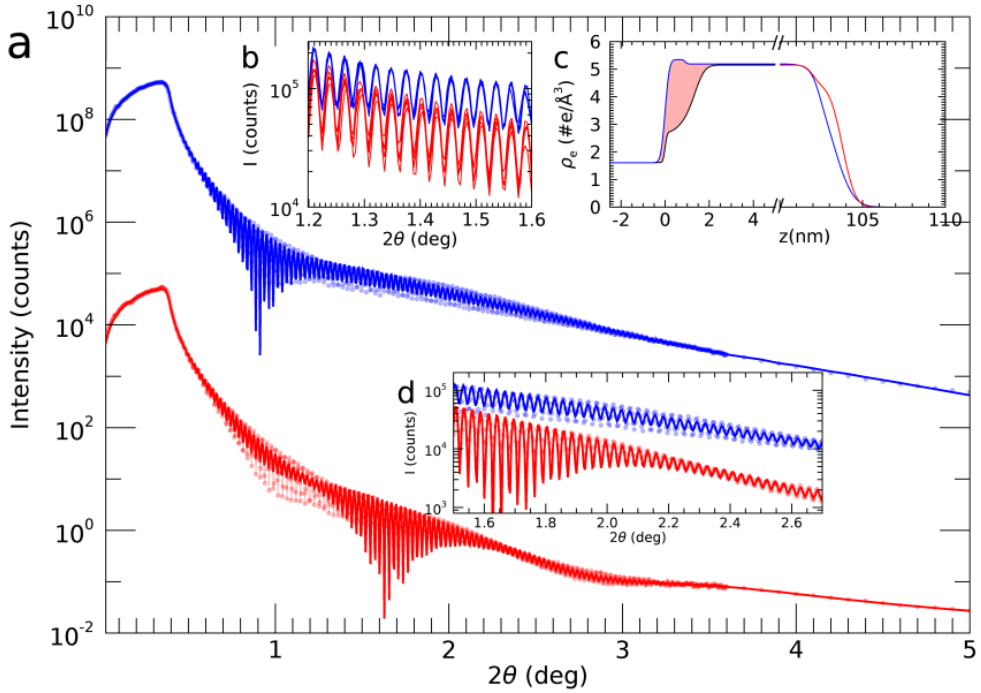

```
  22     0.70002          1         (2, 1)      16676       70015       71453          1
99.9833       -0.981596   608035    335099         76    1.08302e-06   1.6965e+09   52.
  23     0.800018         1         (2, 1)      15718       62296       63782          1
99.9444       -0.974597   607976    334907         76    1.08301e-06   1.6965e+09   54.3
  24     0.900017         1         (2, 1)      13436       51720       53003          1
100.312       -0.990499   610892    335401         76    1.08302e-06   1.6965e+09   56.5
  25     1.00001          1         (2, 1)      11852       39999       41099          0
100.759       -0.987916   613734    336704         76    1.08302e-06   1.6965e+09   58.6
  26     1.10001          1         (2, 1)      10524       35484       36449          0
100.899       -0.977323   613546    337208         76    1.08301e-06   1.6965e+09   60.7
  27     1.20002          1         (2, 1)      10213       30988       31858          0
100.859       -0.979434   613320    337346         76    1.08302e-06   1.6965e+09   62.9
  28     1.30002          1         (2, 1)       7985       24133       24856          0
100.815       -0.973702   613438    337418         76    1.08302e-06   1.6965e+09   65.1
  29     1.40002          1         (2, 1)       5532       16383       16958          0
100.756       -1.00854    613271    337053         76    1.08302e-06   1.6965e+09   67.36
  30     1.50001          1         (2, 1)       4080       11555       11985          0
100.711       -0.974415   612471    336930         76    1.08303e-06   1.6965e+09   69.4
Operation saved in /gpfs/current/raw/run_11017582_00015.fio (fio)
Operation saved in /gpfs/current/raw/run_11017582.dat (Spec)
Scan #15 ended at Thu Oct  5 11:03:09 2023, taking 0:01:11.101551. Dead time 12.8% (motio
Returning to start positions...
Appending 'run_11017582_00015' to /gpfs/current/raw/scicat-datasets-haspp08-11017582.lst
Scan name: /gpfs/current/raw/run_11017582_00015.fio, data from SM
Move om from 1.5e-05 to -0.0707388
Motor om is now at -0.070725
     phis
   7.5365
```

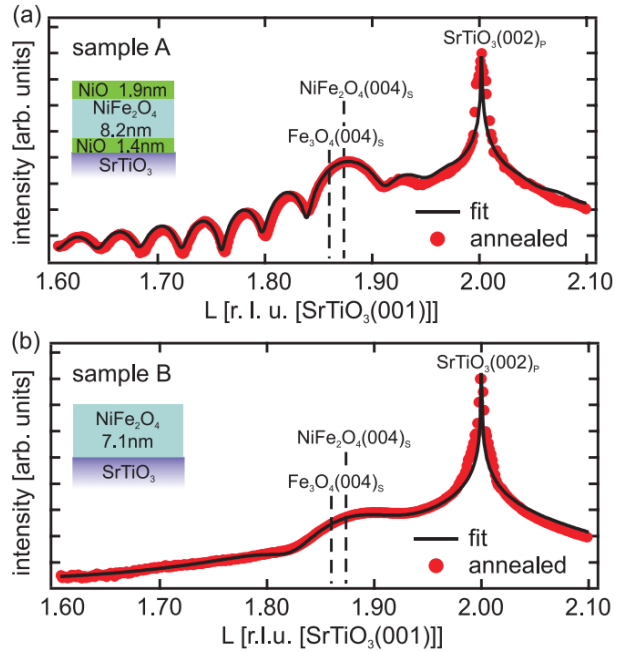
Data after processing

examples



reciprocal space map



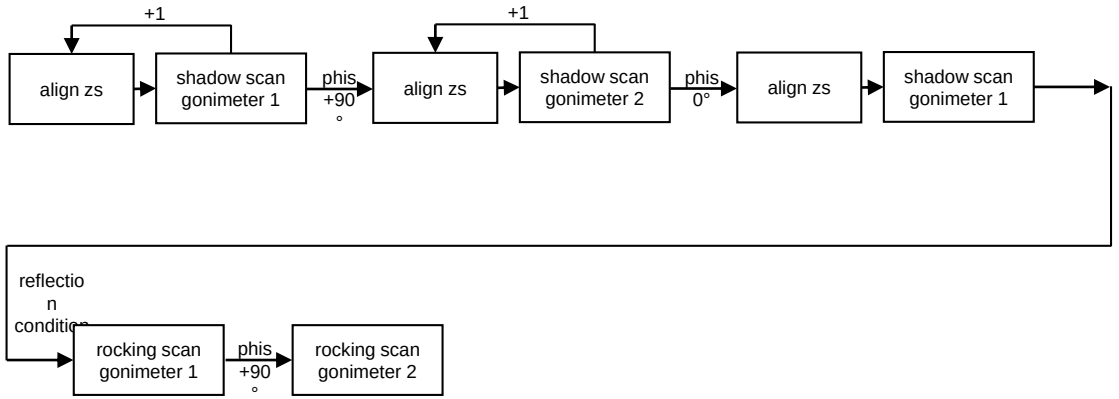


Workflow at the beamline

1. Sample mounting
2. Sample alignment
3. Measurement
4. Change sample condition (e.g. temperature, electric field, pressure, …)

Squence of multiple scans

Example workflow for aligning a surface perpendicular to the inplane rotation



Workflow at the beamline

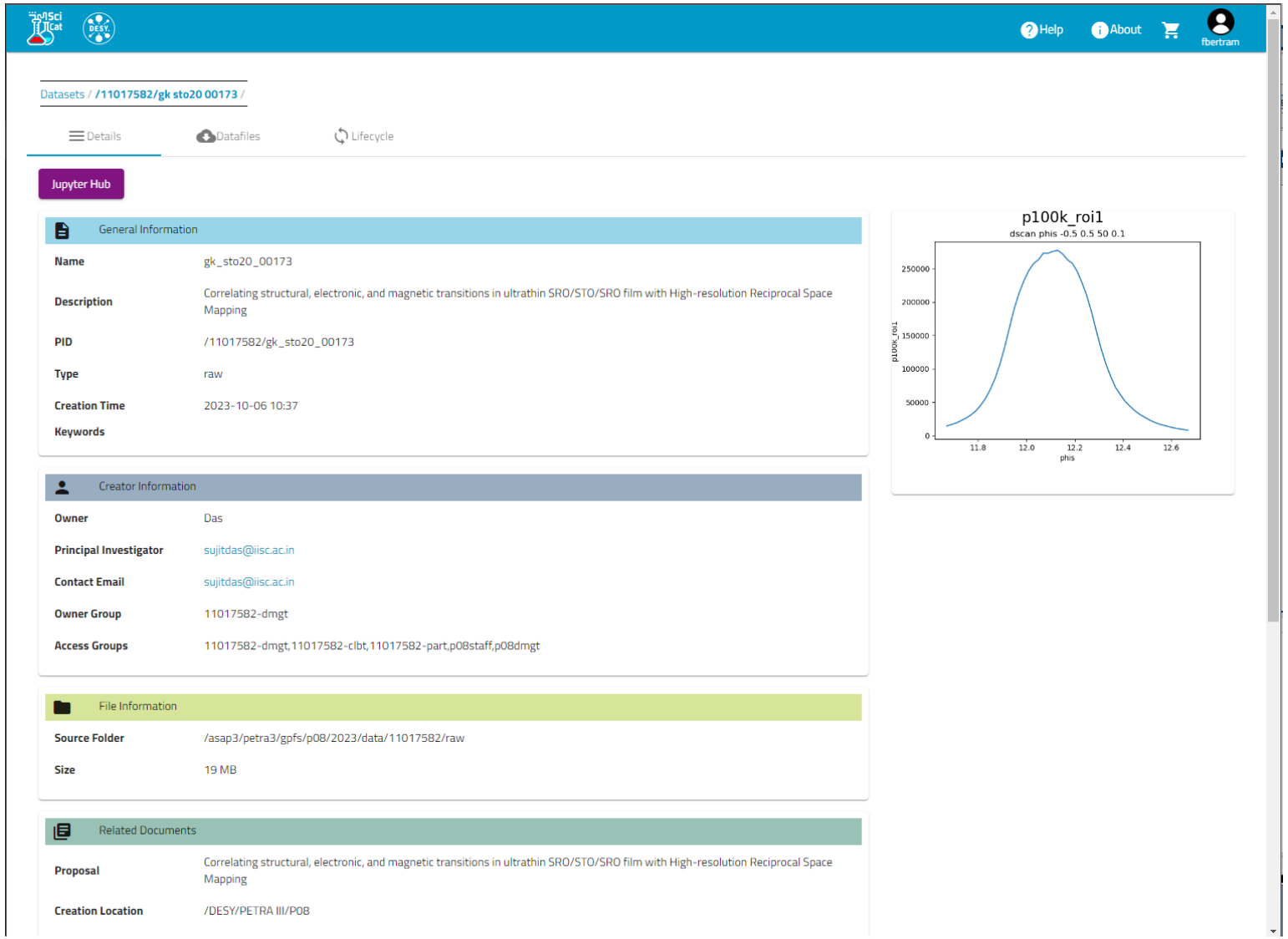
SciCat ingest (implemented by Jan Kotanski, FS-EC)

- On each scan we run „append_scicat_dataset“ in post_scan_hook
  - → appends filename of scan to filelist

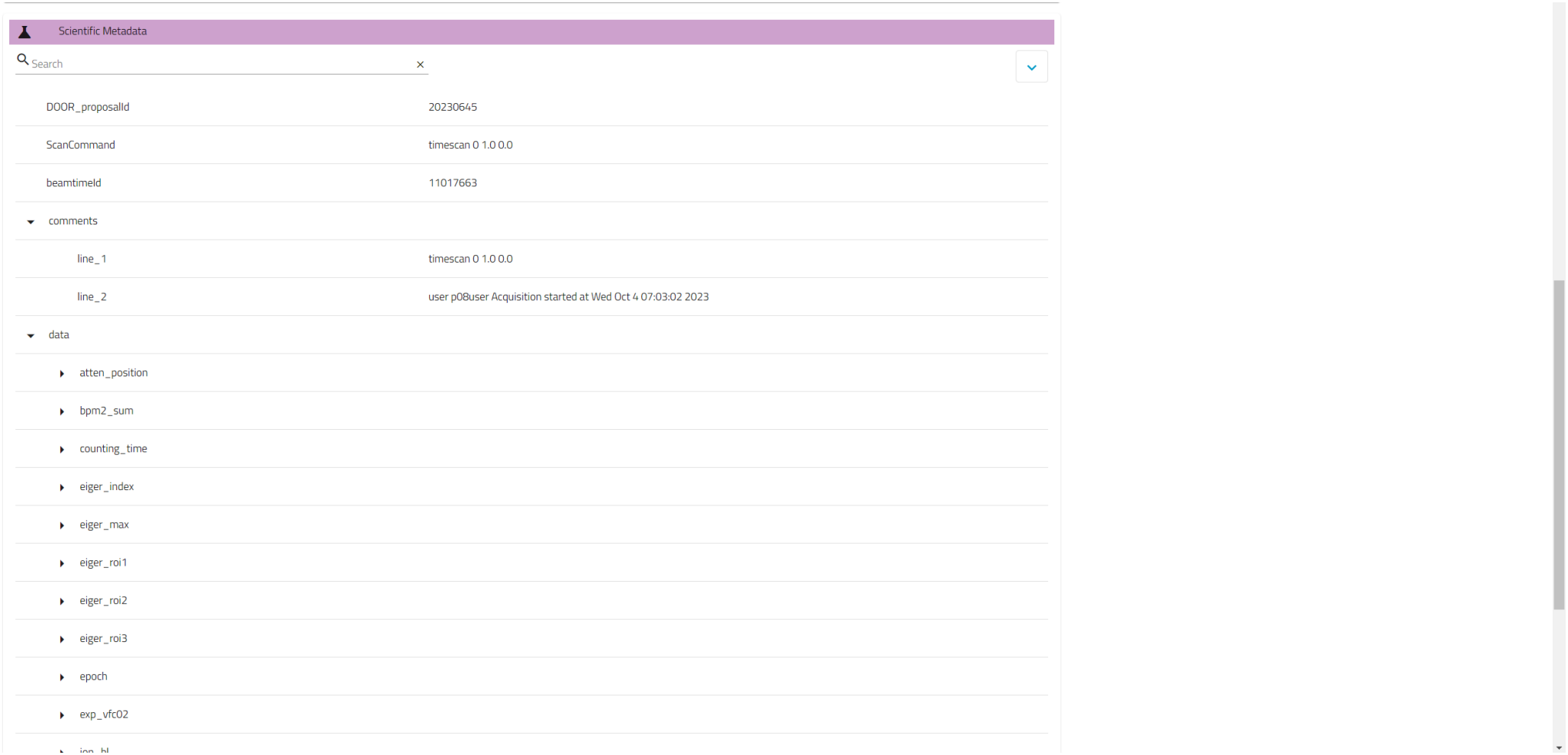
- For each file in filelist a json file is created with information to be feed into scicat

- json file is send to SciCat via API

Typical entries



Typical entries



Typical entries

parameters	
abs	132
anav	5.14532
atten	98.5953
bpm1	7
bpm2	44
bpm3	40
bpm4	43
bsx	0
bsz	-2.17
c2_para	95.5127
c2_perp	10.564
c2_pitch	0.103015
c2_roll	0.145694
c2_tblpitch	61.1219
chi	90
chis	-0.1
dcm_bragg	6.31141
dummymot	1

Problems so far

- Mostly related to web-frontend

- Very unstable
- Frequent logout
- Errors on login
- Data entries sometimes not visible / not accessible
- Slow navigation
- Many entries (>30k), difficult to filter/search/sort
- Custom fields not selectable in dataset table
- Beamtime ID vs Proposal ID (Beamtime ID from DOOR shown as Proposal ID in SciCat)
- Requires DESY/PSX account (procedure for users is very complicated and involves quite some action from beamline)
- (only available from intranet)

Wishlist/questions

- Group entries (e.g. by sample name) for multiple scans
- Flags (alignment, calibration, measurement, etc) with filter option in front end
- Data preview option / thumbnail (plot engine for 1D data?)

  (should be available after data has been moved to tape)
- keywords for datasets/scans, e.g. XRR, XRD, scattering, surface, liquid, solid, powder, …
- Possibility to change grouping, flags and tags afterwards
- After the fact changes of auto-ingested data (e.g. updating thumbnails by processed data, resorting scans into different datasets, change flags, update keywords, …), including change log
- download/staging from “shopping cart”
  - generate tar ball from data available in gpfs for download
  - stage data only available on tape (restore only requested parts but not whole beamtime)

How could the interface look like?

Datasets

measurement calibration alignment

Text

Name

sample

date

proposal

keywords

advanced

Name	sample	date	beamtimeId	Proposal ID	gpfs	
Feosto221220 GID	feosto221220	23-10-08	11017404	I-20230412	true	
Lab6 calibration	LaB6	23-10-07	11017404	I-20230412	true	
beamline alignment	none	23-10-07	11017404	I-20230412	true	
Sample alignemt	…	23-09-08	11016680	I-20230311	false	
X-ray measurement	…	23-09-08	11016680	I-20230311	false	

How could the interface look like?

Datasets

measurement calibration alignment

Text

Name

sample

date

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keywords

advanced

Name	sample	date	beamtimeId	Proposal ID	gpfs	
Feosto221220 GID	feosto221220	23-10-08	11017404	I-20230412	true	
X-ray measurement	…	23-09-08	11016680	I-20230311	false	

How could the interface look like?

Datasets/11017404/Feosto221220 GID

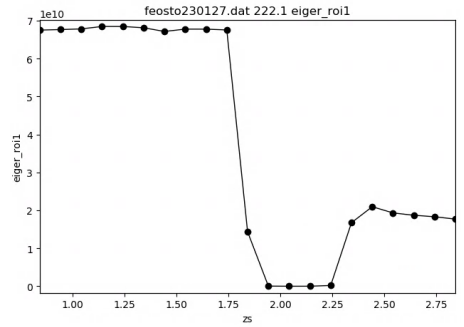
measurement calibration alignment

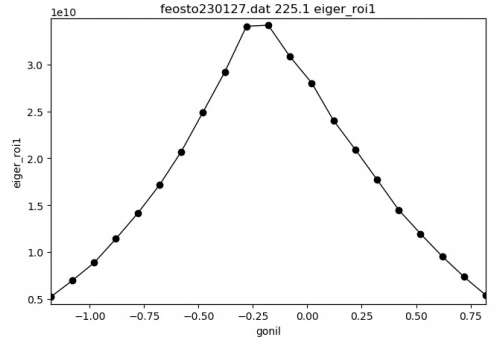
General information

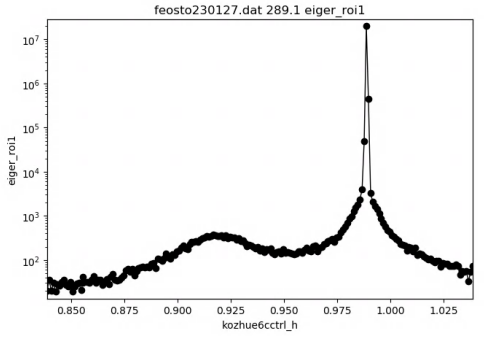
Name	Feosto221220 GID
Description	
Date	23-10-08
sample	FeOSTO221220
keywords	GID, iron oxide, STO(111), thin film
Beamtime ID	11017404
Proposal ID	I-20230412
gpfs	on disk
labbook	link

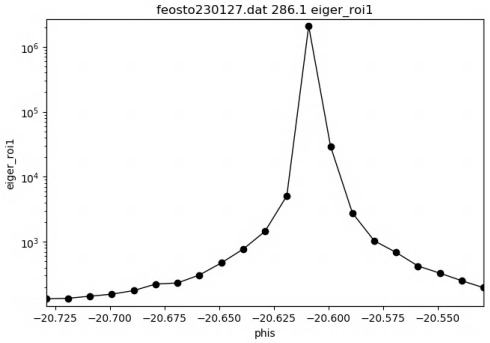
Scientific Metadata

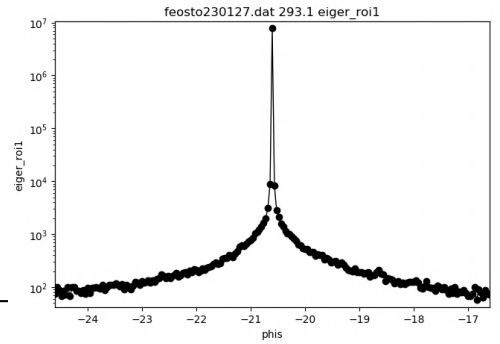
temperature	avg: 30°C; min: 29°C, max: 31°C
pressure	….
photon energy	avg: 15keV; min: 15keV, max: 15keV
….	











How could the interface look like?

Datasets/11017404/Feosto221220 GID

measurement calibration alignment

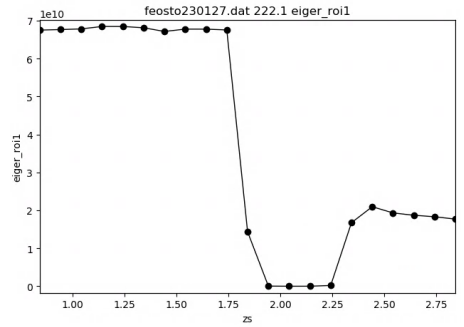
General information

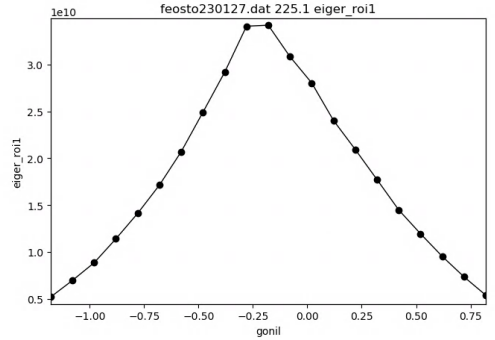
Name	Feosto221220 GID
Description	
Date	23-10-08
sample	FeOSTO221220
keywords	GID, iron oxide, STO(111), thin film
Beamtime ID	11017404
Proposal ID	I-20230412
gpfs	on disk
labbook	link

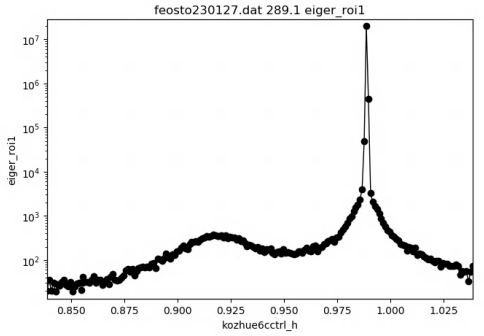
Add to Cart

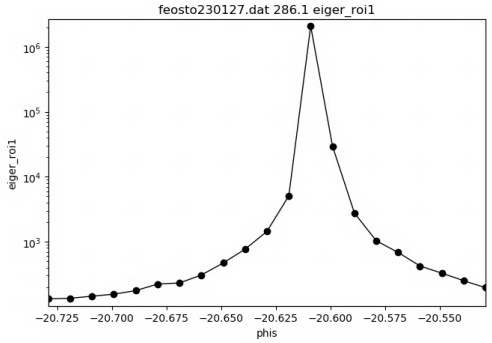
Scans

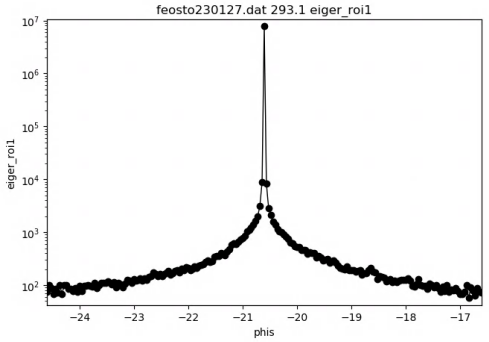
ScanID	cmd	Scan name		
221	dscan zs -1 1 20 1	feosto221220_00221	●	☐
222	dscan om -.2 .2 50 .1	feosto221220_00222	●	☐
230	hklscan 0.9 1.1 0.9 1.1 0.2 0.2 200 10	feosto221220_00230	●	☒
231	dscan phis -5 5 50 1	feosto221220_00231	●	☒
232	Dscan phis -5 5 50 1	feosto221220_00232	●	☒











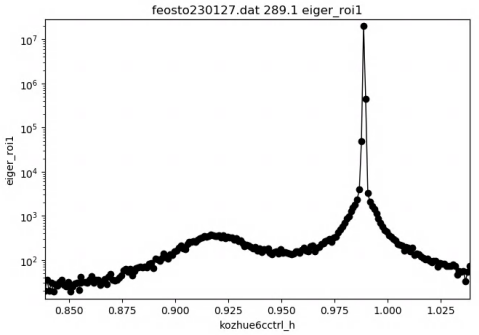
How could the interface look like?

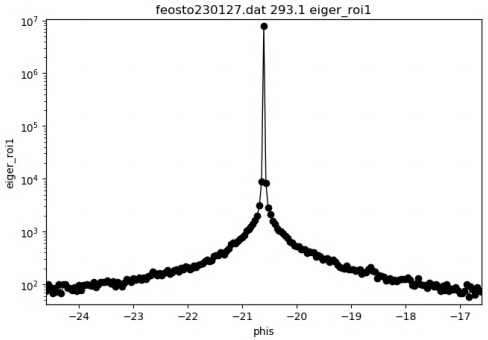
Datasets/11017404/Feosto221220 GID

measurement calibration alignment

General information

Name	Feosto221220 GID
Description	
Date	23-10-08
sample	FeOSTO221220
keywords	GID, iron oxide, STO(111), thin film
Beamtime ID	11017404
Proposal ID	I-20230412
gpfs	on disk
labbook	link





Add to Cart

Scans

ScanID	cmd	Scan name		
230	hklscan 0.9 1.1 0.9 1.1 0.2 0.2 200 10	feosto221220_00230	●	☒
232	dscan phis -5 5 50 1	feosto221220_00232	●	☒