

Example

July 30, 2020

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1 Experimental setup

SIRIUS Beamline : Experiment 123456789

This is an example of JupyterLabBook

- Type: Proposal
- Safety: Yellow
- Date: 12/03/2020-17/03/2020
- Main proposer: Doe
- Local contact: AH
- Users (on site): John Doe, Jane Doe
- Recording directory: /Users/arnaudhemmerle/Documents/Recherche/Analysis/JupyterLabBook/recording/
- Machine:
 - Current: 450 mA
 - Mode: Top-up
- Optics:
 - DCM: Si111
 - MGM: Not used
 - M1: M1-A Pt Track
 - M2: M2 Pt Track
 - M3: No M3
 - M4: M4 Pt Track
- Beam:
 - Fixed/Variable energy: Fixed
 - Energy (keV): 8
 - Wavelength (nm): 0.155
 - Harmonic: 19
 - Polarisation: LH
 - Phase (deg): 0
 - Horizontal focalisation: False
 - Vertical focalisation: True
 - Horizontal beamsize (mm): 2
 - Vertical beamsize (mm): ~0.150
- Monitors and XBPM:
 - mon1:
 - mon2: thick diamond
 - mon3:
 - mon4:
 - Detectors: Pilatus on Delta-Gamma
- Remarks: This is an example.

2 Beamline alignment

Here we show functions used during beamline alignment.

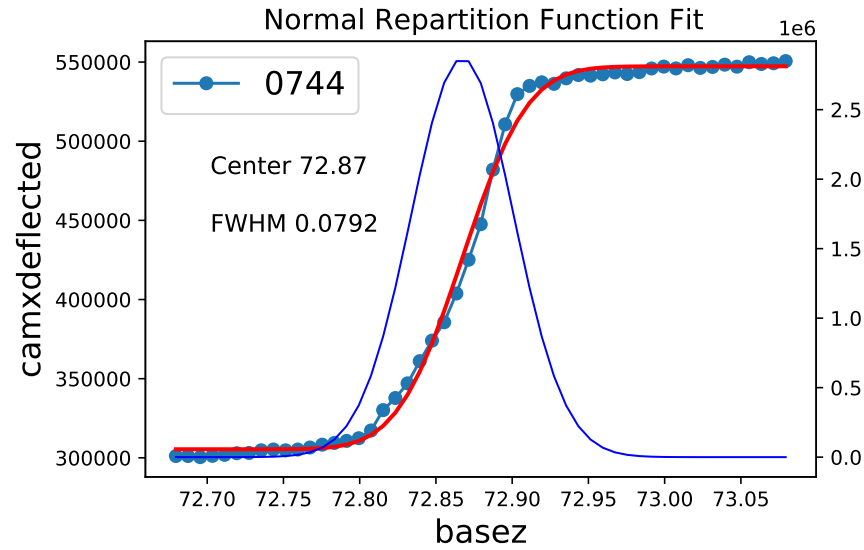
LaTeX formula can be used:

$$\frac{786 - 558}{2 \times 2069} \times 0.0355 = 1.9 \text{ mrad}$$

2.1 Subsection

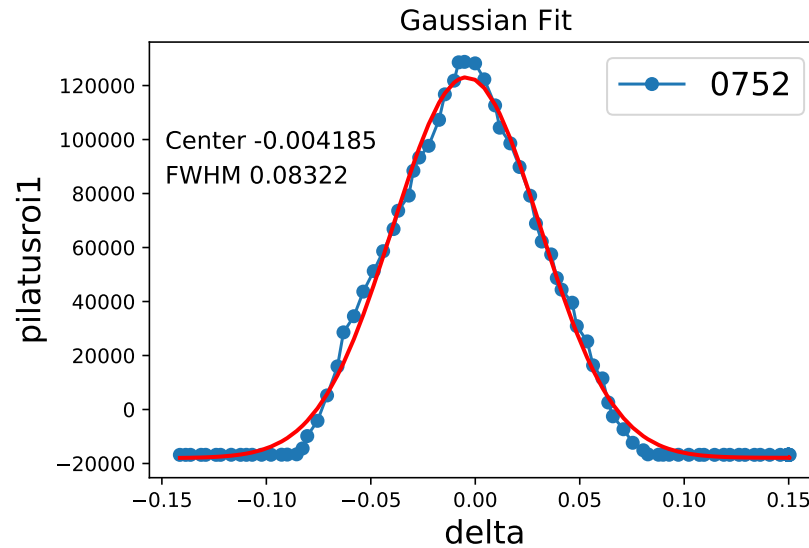
2.1.1 SIRIUS_2020_03_11_0744: dscan basez -.2 .2 50 .1

Fit with erf function.

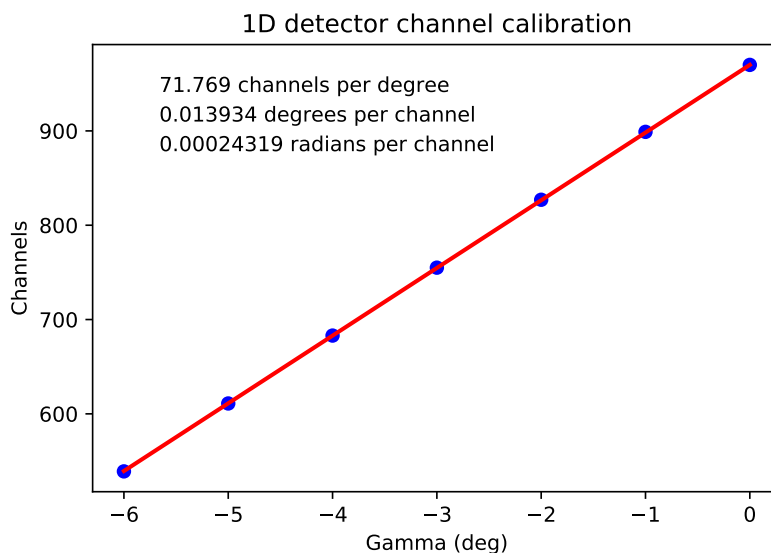


2.1.2 SIRIUS_2020_03_11_0752: One can edit the scan info here as well

Fit with a gaussian.



2.2 Calibration thetaz



3 GIXD

3.0.1 SIRIUS_2020_03_12_0756: continuous_ascan delta -24 -19 100 5

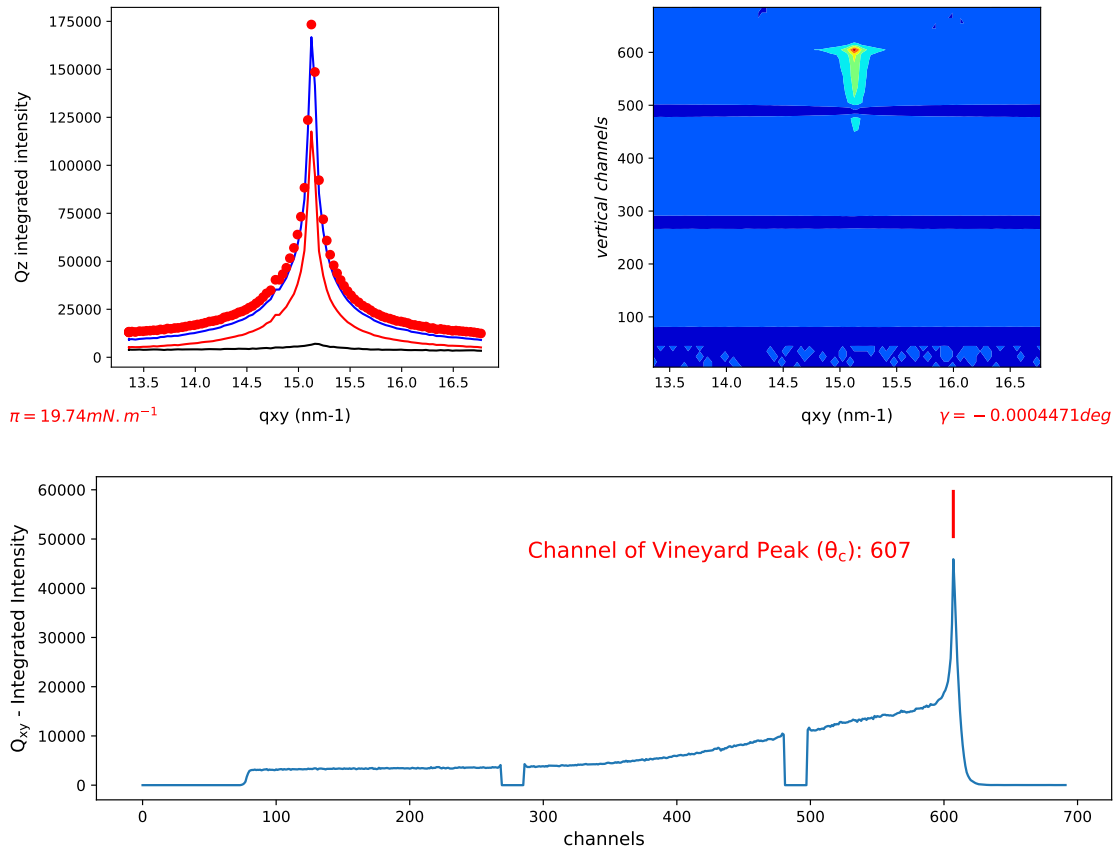
Extraction of the Vineyard.

- Open Nexus Data File :

```
recording/SIRIUS_2020_03_12_0756.nxs
. Number of data points: 101
. Available Counters:
  0 -----> delta
  1 -----> zs
  2 -----> gamma
  3 -----> hu36energy
  4 -----> xs
  5 -----> energydcm
  6 -----> current
  7 -----> mon2
  8 -----> surfacepressure
  9 -----> areapermolecule
 10 -----> qxy
 11 -----> pilatus
 12 -----> pilatusroi1
 13 -----> integration_time
 14 -----> sensorsRelTimestamps
 15 -----> sensorsTimestamps
. Pilatus data found, (column 11, alias pilatus)
. qxy data found, (column 10, alias qxy)
. Surface pressure data found, mean value 19.74 ± 0.006119 mN/m
. Area per molecule data found, mean value 0.3557 ± 3.944e-05 nm2 per
```

molecule

. Gamma motor data found, mean value -0.0004471 deg
SIRIUS_2020_03_12_0756.nxs



Data not saved. To save data, run a GIXD on the scan.
Channel0: 607

3.0.2 SIRIUS_2020_03_12_0756: continuous_ascan delta -24 -19 100 5

Classic GIXD with:

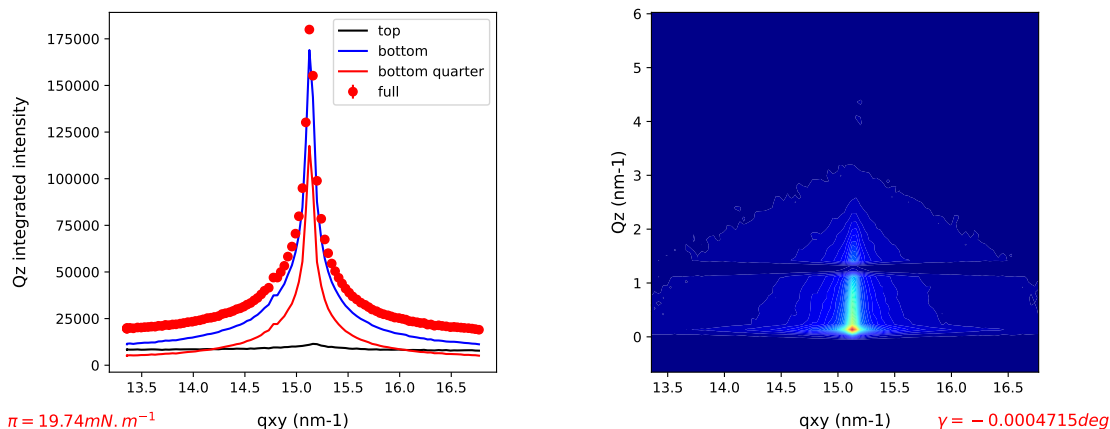
$$q_{xy} = \frac{4\pi}{\lambda} \sin\left(\frac{2\theta}{2}\right)$$

Generates:

- SIRIUS_2020_03_12_0756_1D_qz.dat for each binning
- SIRIUS_2020_03_12_0756_1D.dat
- SIRIUS_2020_03_12_0756_1D.mat for each binning
- SIRIUS_2020_03_12_0756_1D.moy for each binning

. Absorbers: 29 - Vide

SIRIUS_2020_03_12_0756.nxs



3.0.3 SIRIUS_2020_03_12_0756: continuous_ascan delta -24 -19 100 5

It is possible to print all info on the scan and the counters.

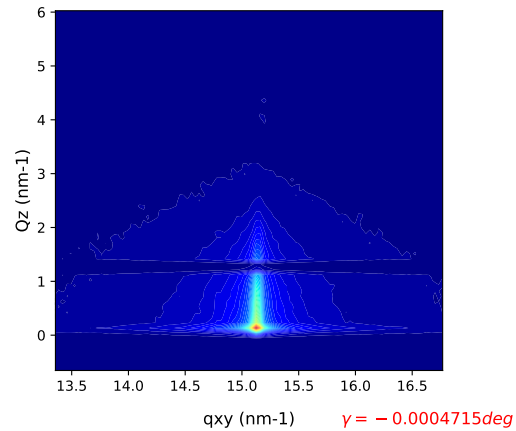
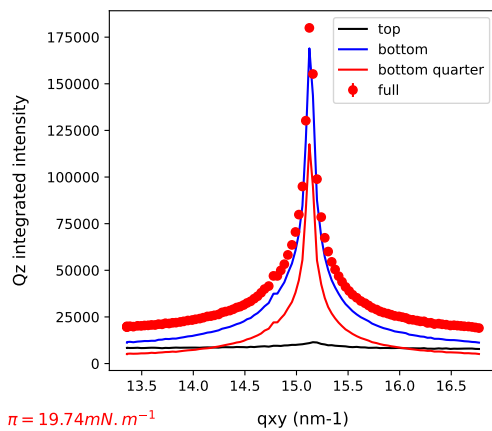
- Open Nexus Data File :

```
recording/SIRIUS_2020_03_12_0756.nxs
. Number of data points: 101
. Available Counters:
    0 -----> delta
    1 -----> zs
    2 -----> gamma
    3 -----> hu36energy
    4 -----> xs
    5 -----> energydcm
    6 -----> current
    7 -----> mon2
    8 -----> surfacepressure
    9 -----> areapermolecule
   10 -----> qxy
   11 -----> pilatus
   12 -----> pilatusroi1
   13 -----> integration_time
   14 -----> sensorsRelTimestamps
   15 -----> sensorsTimestamps
. Absorbers: 29 - Vide
. Pilatus data found, (column 11, alias pilatus)
. qxy data found, (column 10, alias qxy)
. Valid data between points 0 and 100
. Surface pressure data found, mean value 19.74 ± 0.006163 mN/m
. Area per molecule data found, mean value 0.3557 ± 3.866e-05 nm2 per
molecule
. Gamma motor data found, mean value -0.0004715 deg
. Original, non binned matrix saved in:
working/SIRIUS_2020_03_12_0756_1D.mat
```

```

. Scalar data saved in:
working/SIRIUS_2020_03_12_0756_1D.dat
. Qz values saved in:
working/SIRIUS_2020_03_12_0756_1D_qz.dat10
. Binned matrix saved in:
working/SIRIUS_2020_03_12_0756_1D.mat10
. XYZ data saved in:
working/SIRIUS_2020_03_12_0756_1D.moy10
. Qz values saved in:
working/SIRIUS_2020_03_12_0756_1D_qz.dat20
. Binned matrix saved in:
working/SIRIUS_2020_03_12_0756_1D.mat20
. XYZ data saved in:
working/SIRIUS_2020_03_12_0756_1D.moy20
. Qz values saved in:
working/SIRIUS_2020_03_12_0756_1D_qz.dat40
. Binned matrix saved in:
working/SIRIUS_2020_03_12_0756_1D.mat40
. XYZ data saved in:
working/SIRIUS_2020_03_12_0756_1D.moy40
SIRIUS_2020_03_12_0756.nxs

```

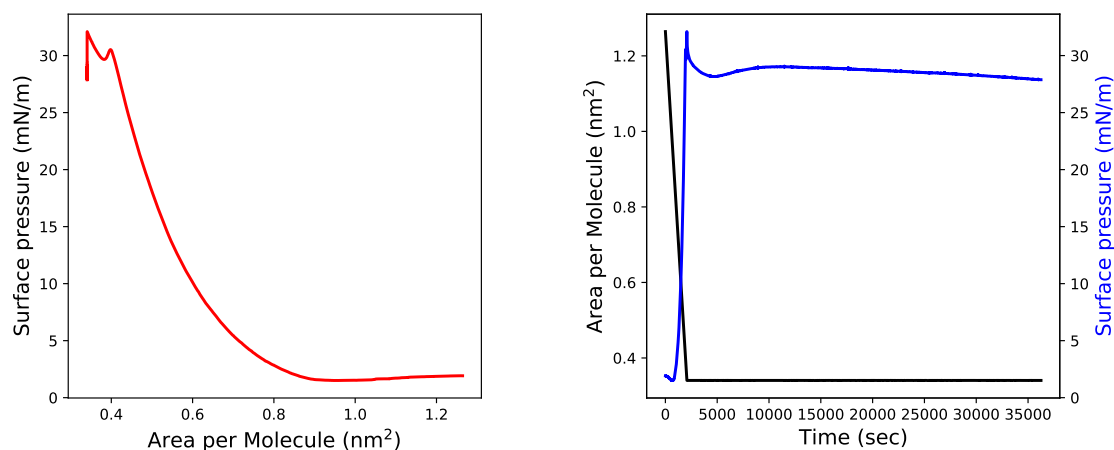


4 Isotherm

4.0.1 SIRIUS_Isotherm_2019_02_17_01544: isotherm 1.97 46 35000 1

Plot the isotherm. Generates SIRIUS_Isotherm_2019_02_17_01544.dat

SIRIUS_Isotherm_2019_02_17_01544

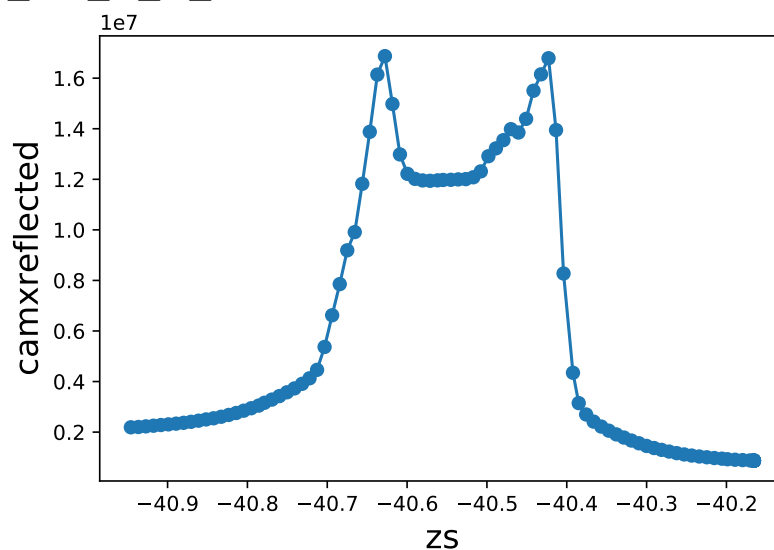


5 1D plot

5.0.1 SIRIUS_2020_03_12_0760: run cont_regh.ipy

Add a 1D plot by clicking on "Add plot to report".

Generates SIRIUS_2020_03_12_0760.dat



6 GIXS

6.0.1 SIRIUS_2019_11_07_00325: tscan 10 10

GIXS: q_z vs q_{xy} .

Image and profiles with the approximation $q_{xy} = \frac{4\pi}{\lambda} \sin\left(\frac{2\theta}{2}\right)$.

Generates:

- SIRIUS_2019_11_07_00325_pilatus_sum.tiff

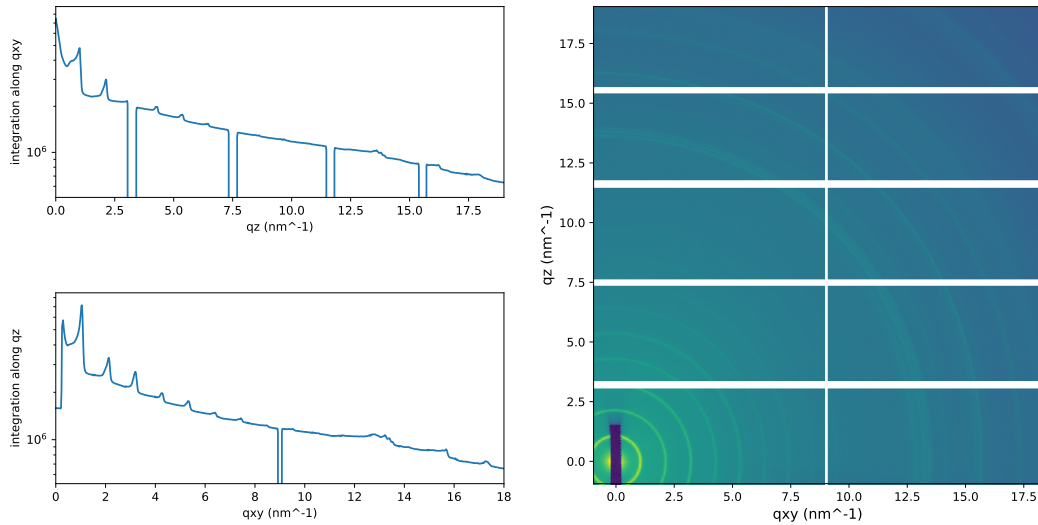
- SIRIUS_2019_11_07_00325_pilatus_sum.mat
- SIRIUS_2019_11_07_00325_integrated_qz.dat
- SIRIUS_2019_11_07_00325_integrated_qxy.dat

6.0.2 SIRIUS_2019_11_07_00325: tscan 10 10

```
. Absorbers: 29 - Vide

. No gamma found! gamma = 0
. No delta found! delta = 11.578
```

SIRIUS_2019_11_07_00325.nxs



7 Plot pilatus

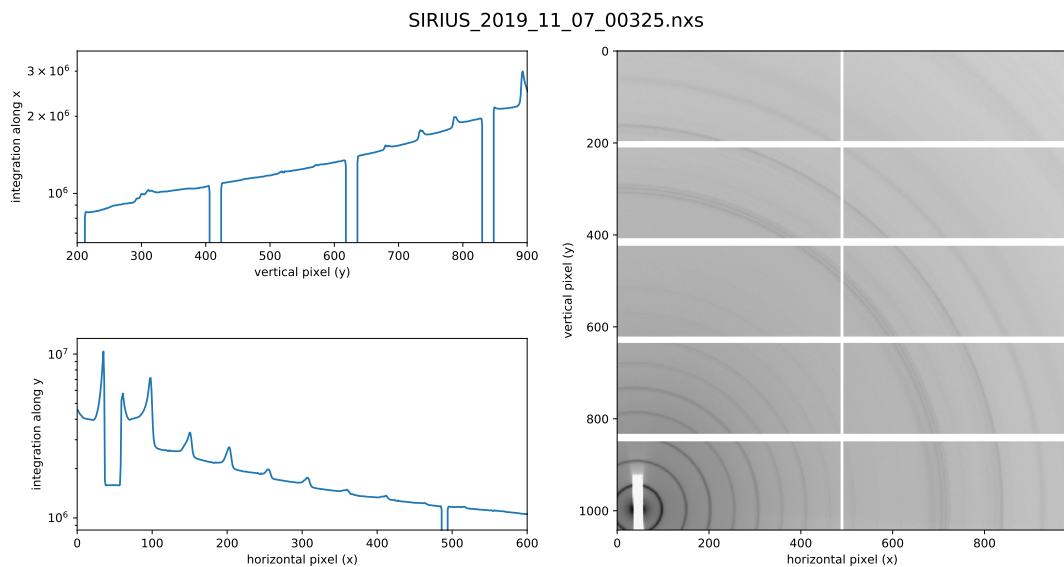
7.0.1 SIRIUS_2019_11_07_00325: tscan 10 10

Plot the sum of the images from the Pilatus (time integration).

Generates:

- SIRIUS_2019_11_07_00325_pilatus_sum.tiff
- SIRIUS_2019_11_07_00325_pilatus_sum.mat
- SIRIUS_2019_11_07_00325_integrated_x.dat
- SIRIUS_2019_11_07_00325_integrated_y.dat

```
. Absorbers: 29 - Vide
```



8 XRF

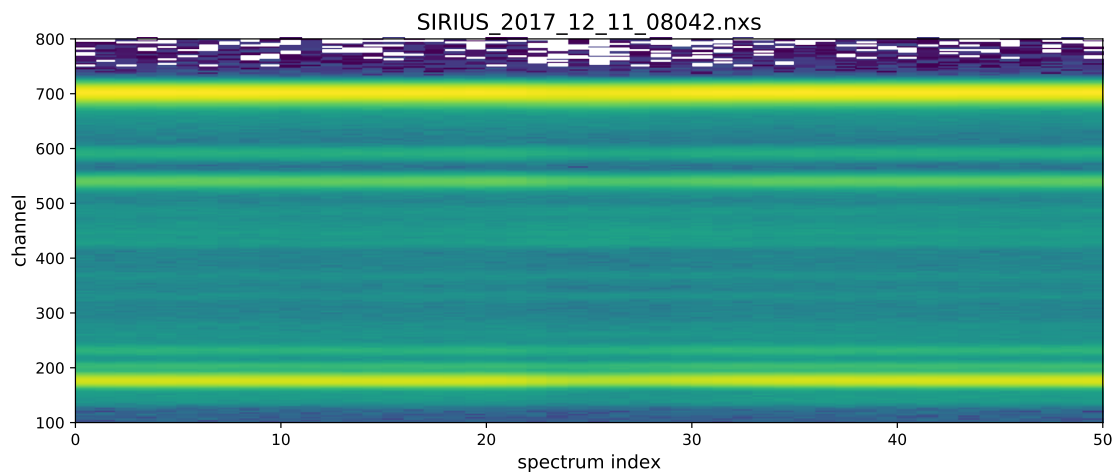
8.0.1 SIRIUS_2017_12_11_08042: run xsw7.ipynb

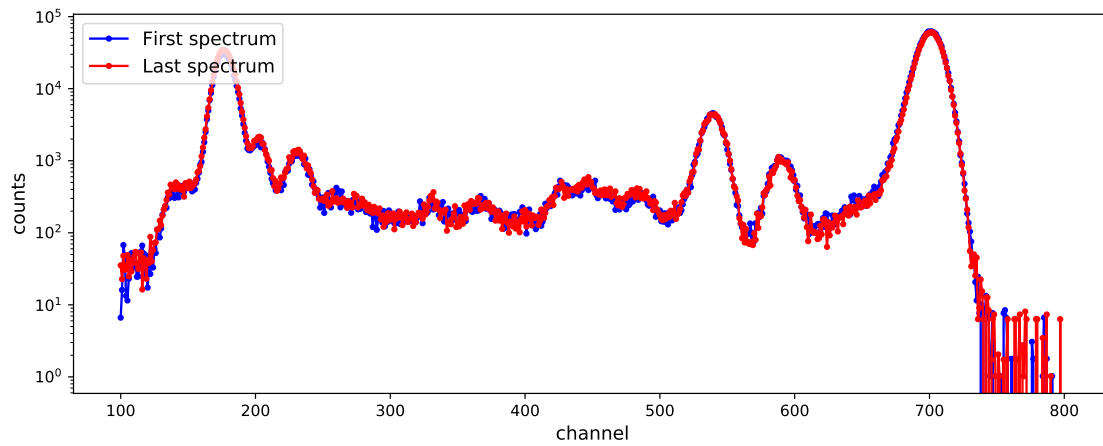
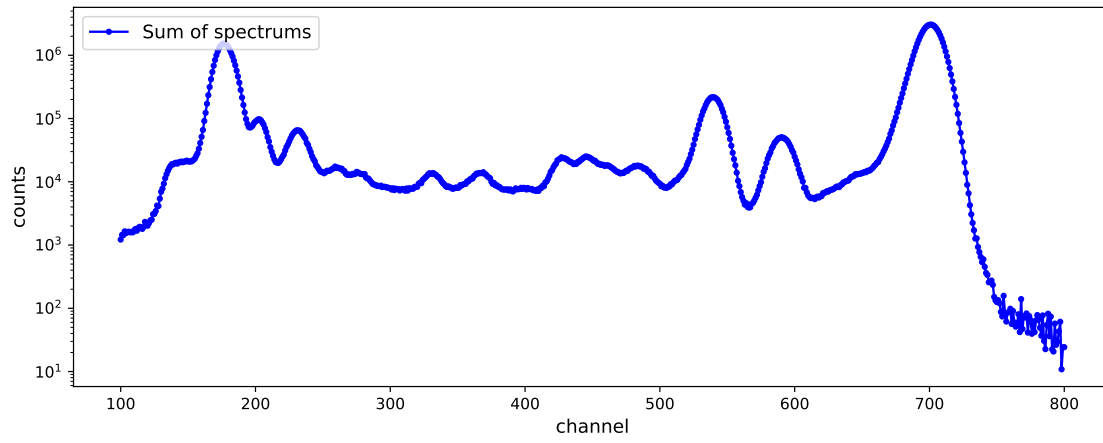
Plot XRF from the 4-elements detector, in channels and without peak identification.

Generates:

- SIRIUS_2017_12_11_08042_fluospectrum.mat for each element
- SIRIUS_2017_12_11_08042.dat

. Absorbers: Al 200micron





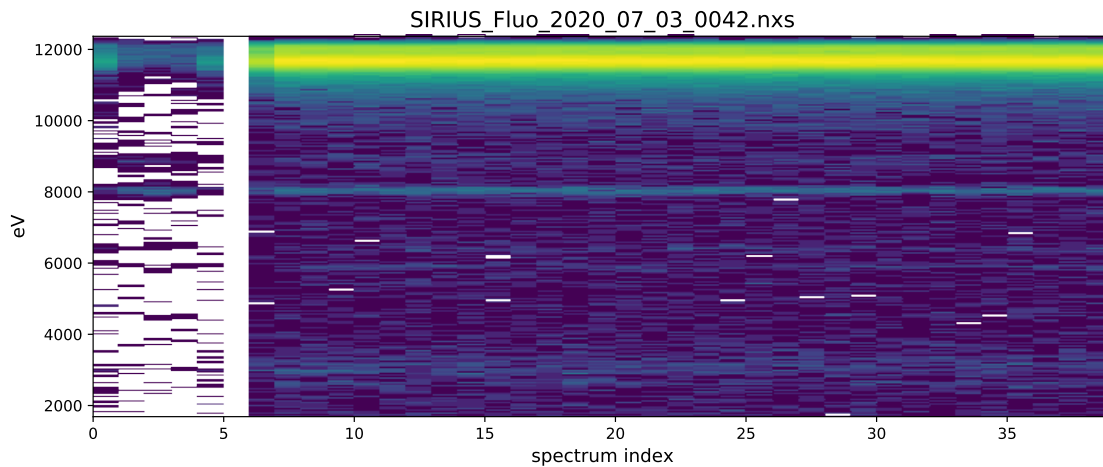
8.0.2 SIRIUS_Fluo_2020_07_03_0042: tscan 500 30

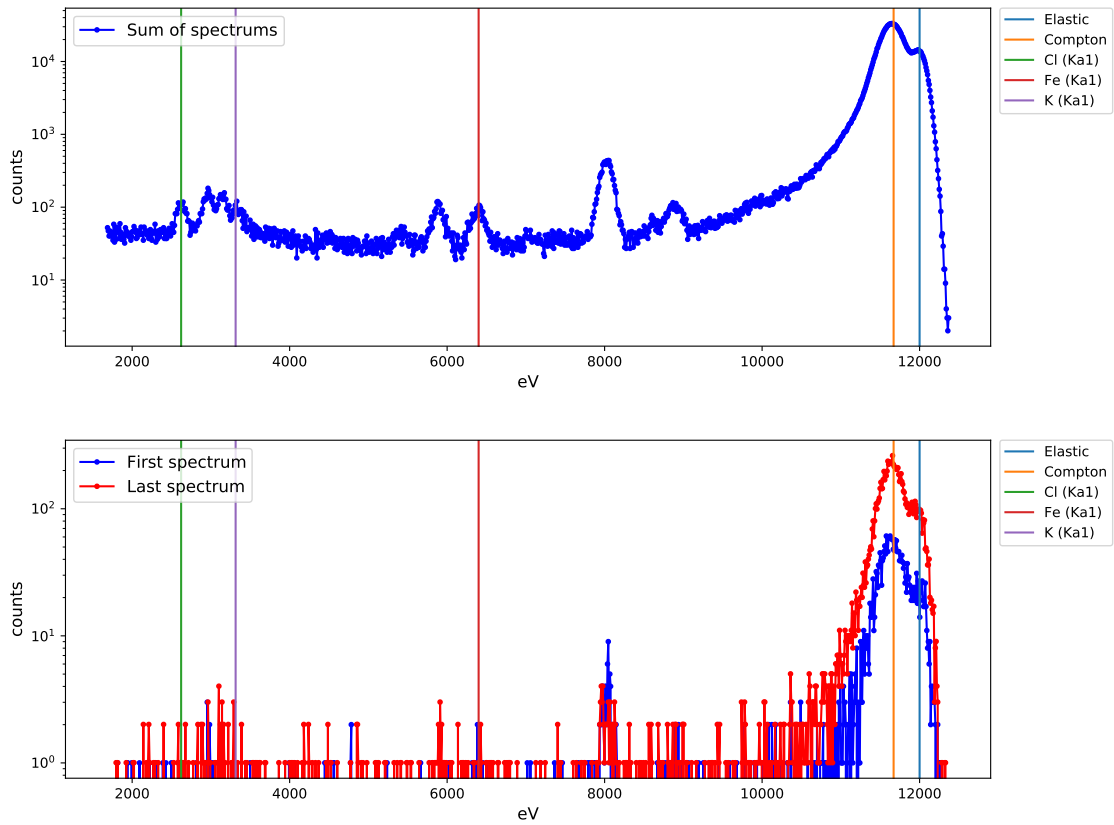
Plot XRF from the 1-element detector, in eVs and with peak identification.

Generates:

- SIRIUS_Fluo_2020_07_03_0042_fluospectrum04.mat
- SIRIUS_Fluo_2020_07_03_0042.dat

. Absorbers: Al 800micron





9 Insert script

Script inserted (with automatic scan numbering) using "Insert script".

9.0.1 script_with_loop.ipynb

```
%shopen
%amove delta -40
%run reset_motors.ipynb
%amove delta -35
%continuous_ascan delta -35 -25 250 5 #123
%run reset_motors.ipynb
for i in range(4):
    %amove delta -20
    %continuous_ascan delta -10 -3 175 5 #124 #126 #128 #130
    %run reset_motors.ipynb
    %run cont_regh_abs.ipynb #125 #127 #129 #131
for i in range(3):
    %amove delta -20
    %continuous_ascan delta -10 -3 175 5 #132 #135 #138
    %run reset_motors.ipynb
    %run cont_regh_abs.ipynb #133 #136 #139
    %run cont_regh_abs.ipynb #134 #137 #140
for i in range(2):
```

```

%amove delta -20
%tscan 10 100 #141 #142

%continuous_ascan delta -35 -25 250 5 #143
%amove delta -40
%shclose

```

10 Insert positions

Positions extracted from the logs, using ’’Insert positions’’.

10.0.1 wm zs

zs
-40.9178

10.0.2 wm diffracto

deltacodeur	euchi	euth	euphi	kappa_h	kappa_k
	1.00196	-89.57961	90.42039	-0.00580	-0.08252
Degrees	deg	deg	deg		

kappa_l	qxy	qxy0	qz	basezPoint	basezTrait
-0.18486	2.0556	23.82	-0.92	-15.7275	-15.7274
	nm-1	nm-1	nm-1		

basezPlan	basezPoint	basezTrait	basepitch	baseroll	basex
71.1257	71.1257	71.1257	-0.0000	0.000	-15.727
			mmrad	mmrad	mm

baseyaw	basez	alphax	alphay	delta	delta0
-0.000	71.126	0.2998	0.2000	-2.9110	-34.2322
mmrad	mm				

deltaa	etaa	gamma	kappav	mu	kphi
0.0000	0.0000	1.2997	1.3080	-179.9997	0.0000

thetaa	thetah	komega	xs	ky	ys
0.0000	0.0185	0.0000	0.0000	-0.1000	0.0000

kz	zs	kx
0.0000	-41.9999	-0.1000

11 Insert commands

Commands extracted from the logs, using ‘‘Insert commands’’.

```

Wed, 11 Mar 2020 13:59:25 dmove m4tz 1
Wed, 11 Mar 2020 13:59:29 ct 1
Wed, 11 Mar 2020 13:59:37 amove m4pitch -.02
Wed, 11 Mar 2020 13:59:39 ct 1
Wed, 11 Mar 2020 13:59:50 dmove m4tz -.5
Wed, 11 Mar 2020 13:59:53 ct 1
Wed, 11 Mar 2020 13:59:56 dmove m4tz -.5
Wed, 11 Mar 2020 14:00:00 ct 1
Wed, 11 Mar 2020 14:00:12 dscan m4tz -.5 1.5 50 .1 #679
Wed, 11 Mar 2020 14:01:47 sigmoid_dscan m4tz -.4 .4 50 .1 #680
Wed, 11 Mar 2020 14:03:41 amove m4tz PEAK
Wed, 11 Mar 2020 14:03:50 dscan m4pitch -.5 .5 50 .1 #681
Wed, 11 Mar 2020 14:05:04 sigmoid_dscan m4tz -.4 .4 50 .1 #682

```

12 Convert logs

Human-readable logs generated in the folder /working/readable_logs/ by clicking on ‘‘Convert logs’’.

13 Export to pdf

PDF generated by clicking on ‘‘Export to pdf’’.