Example

July 13, 2020

Contents

1 Experimental setup

SIRIUS Beamline : Experiment 123456789

This is an example of JupyLabBook

- 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/JupyLabBook/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

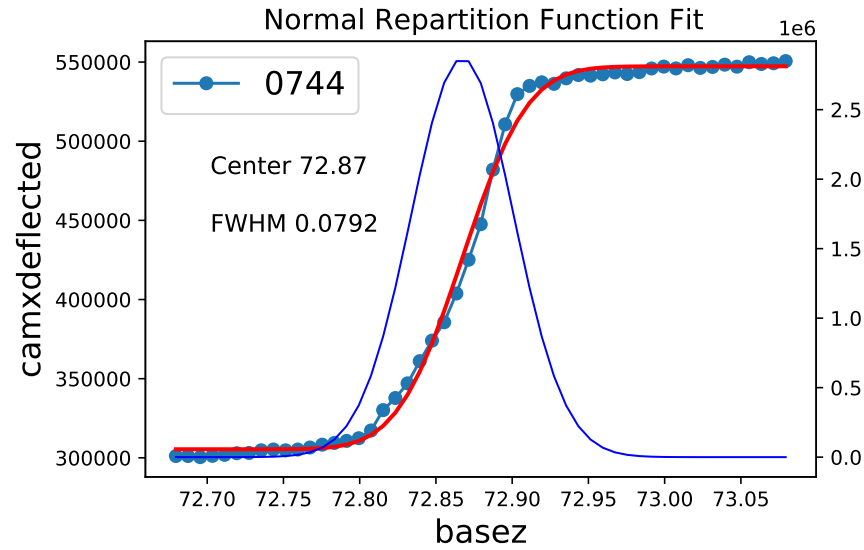Here we show functions used during beamline aligment.

LaTeX formula can be used:

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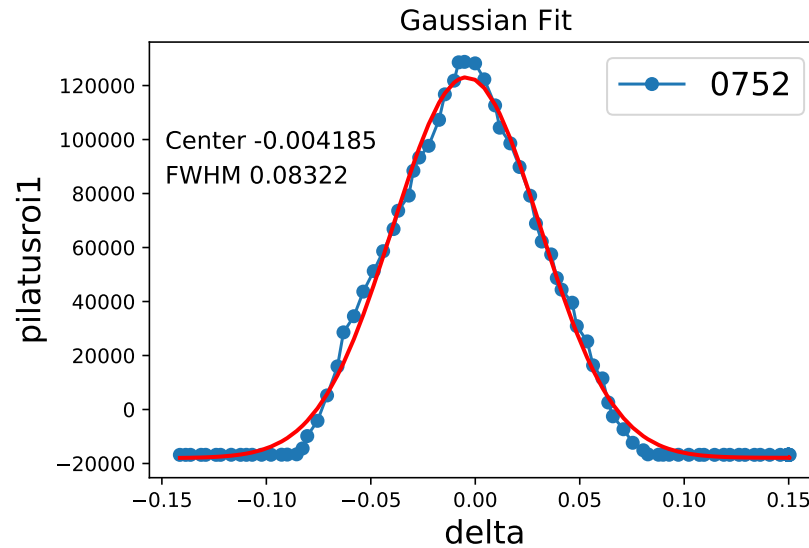
2.1   Subsection

2.1.1   SIRIUS_2020_03_11_0744: dscan basez -.2 .2 50 .1
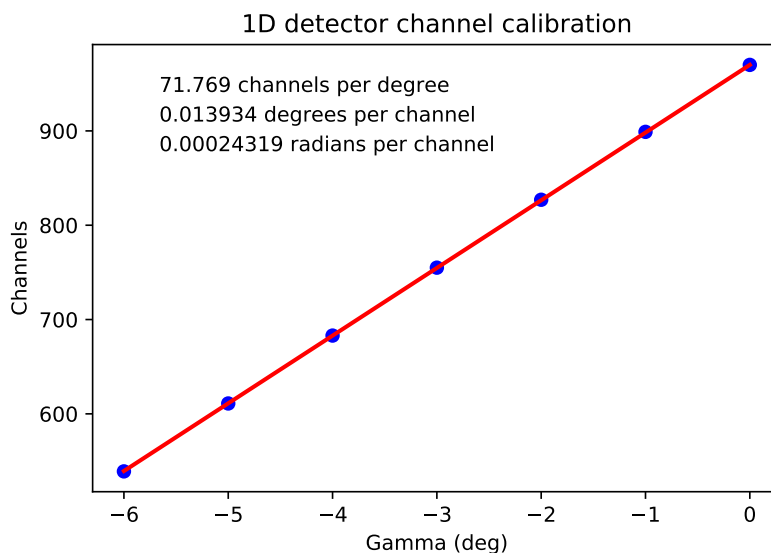
Fit with erf function.

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

1D detector channel calibration

71.769 channels per degree
0.013934 degrees per channel
0.00024319 radians per channel

Channels (y-axis) vs Gamma (deg) (x-axis)

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 :
     /Users/arnaudhemmerle/Documents/Recherche/Analysis/JupyLabBook/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
```
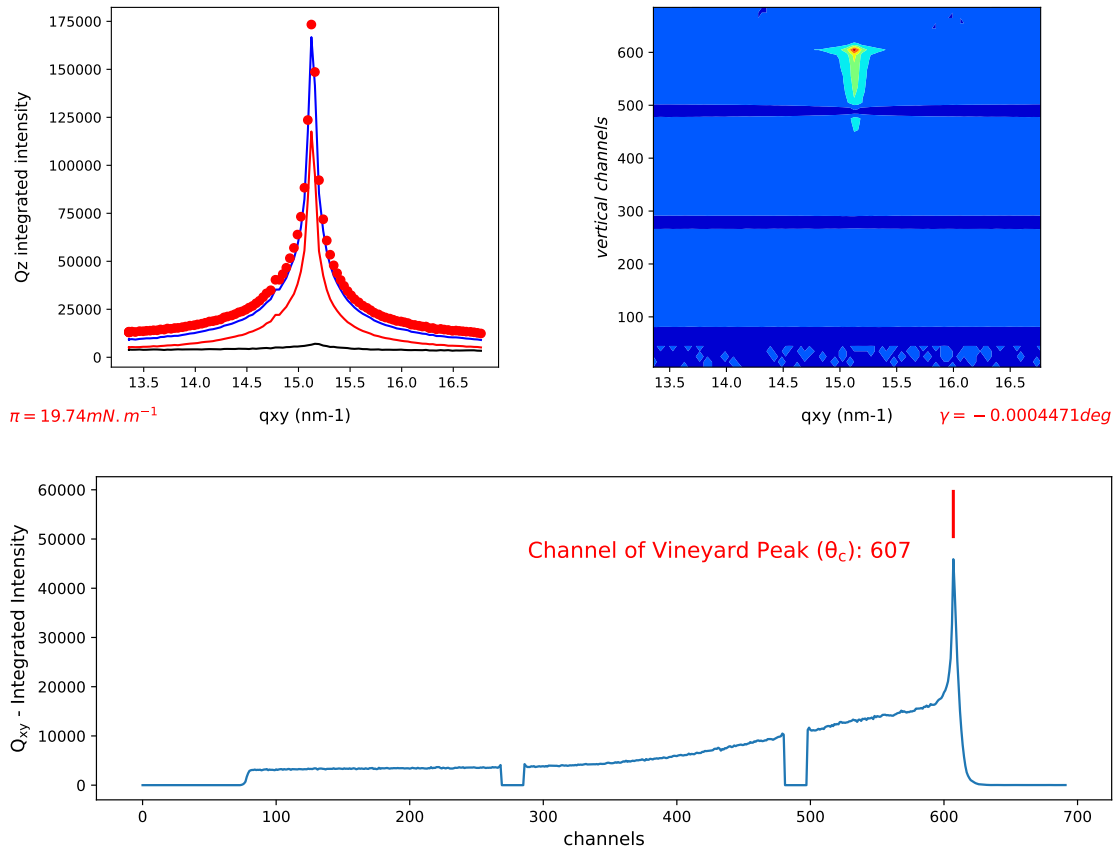
```
molecule
       . Gamma motor data found, mean value -0.0004471 deg
```


SIRIUS_2020_03_12_0756.nxs

$\pi = 19.74 mN.m^{-1}$

$\gamma = -0.0004471 deg$

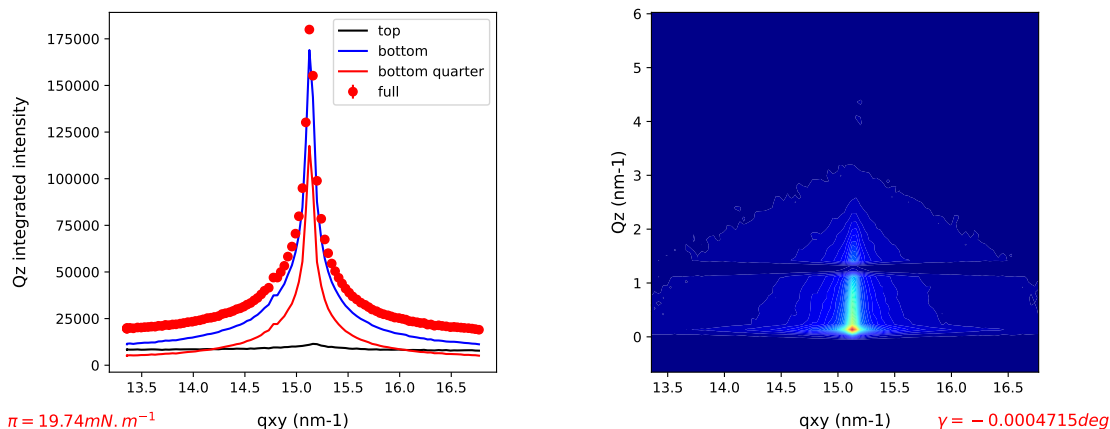### 3.0.2 SIRIUS_2020_03_12_0756: continuous_ascan delta -24 -19 100 5

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

$\pi = 19.74 mN. m^{-1}$

$\gamma = -0.0004715 deg$

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.

GIXD without the approximation on q_{xy}. Generates the same files as with classic GIXD.

- **Open Nexus Data File :**
    /Users/arnaudhemmerle/Documents/Recherche/Analysis/JupyLabBook/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
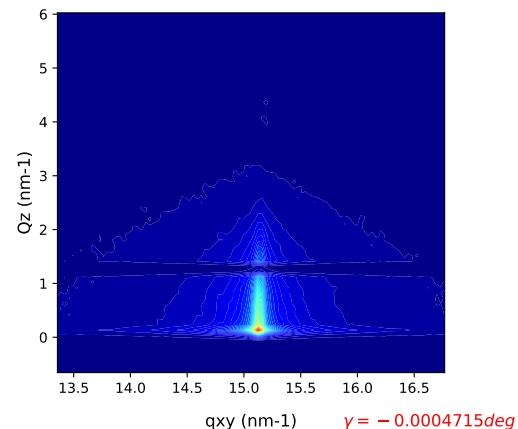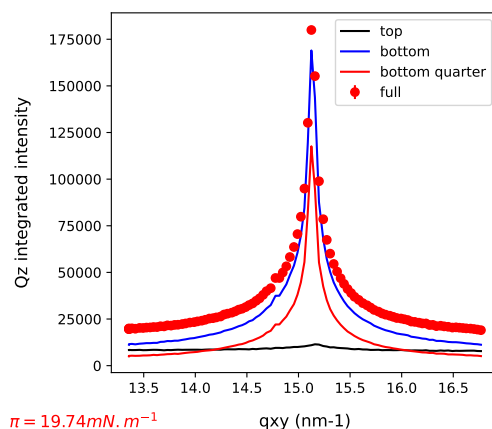molecule
   . Gamma motor data found, mean value -0.0004715 deg

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```
. For more details on the geometry, see:
        -Fig.2 in doi:10.1107/S0909049512022017
        -Slide 4 in http://gisaxs.com/files/Strzalka.pdf
. Original, non binned matrix saved in:
    /Users/arnaudhemmerle/Documents/Recherche/Analysis/JupyLabBook/working/
SIRIUS_2020_03_12_0756_1D.mat
. Scalar data saved in:
    /Users/arnaudhemmerle/Documents/Recherche/Analysis/JupyLabBook/working/
SIRIUS_2020_03_12_0756_1D.dat
. Qz values saved in:
    /Users/arnaudhemmerle/Documents/Recherche/Analysis/JupyLabBook/working/S
IRIUS_2020_03_12_0756_1D_qz10.dat
. Binned matrix saved in:
    /Users/arnaudhemmerle/Documents/Recherche/Analysis/JupyLabBook/working/
SIRIUS_2020_03_12_0756_1D.mat10
. XYZ    data saved in:
    /Users/arnaudhemmerle/Documents/Recherche/Analysis/JupyLabBook/working/
SIRIUS_2020_03_12_0756_1D.moy10
. Qz values saved in:
    /Users/arnaudhemmerle/Documents/Recherche/Analysis/JupyLabBook/working/S
IRIUS_2020_03_12_0756_1D_qz20.dat
. Binned matrix saved in:
    /Users/arnaudhemmerle/Documents/Recherche/Analysis/JupyLabBook/working/
SIRIUS_2020_03_12_0756_1D.mat20
. XYZ    data saved in:
    /Users/arnaudhemmerle/Documents/Recherche/Analysis/JupyLabBook/working/
SIRIUS_2020_03_12_0756_1D.moy20
. Qz values saved in:
    /Users/arnaudhemmerle/Documents/Recherche/Analysis/JupyLabBook/working/S
IRIUS_2020_03_12_0756_1D_qz40.dat
. Binned matrix saved in:
    /Users/arnaudhemmerle/Documents/Recherche/Analysis/JupyLabBook/working/
SIRIUS_2020_03_12_0756_1D.mat40
. XYZ    data saved in:
    /Users/arnaudhemmerle/Documents/Recherche/Analysis/JupyLabBook/working/
SIRIUS_2020_03_12_0756_1D.moy40
```
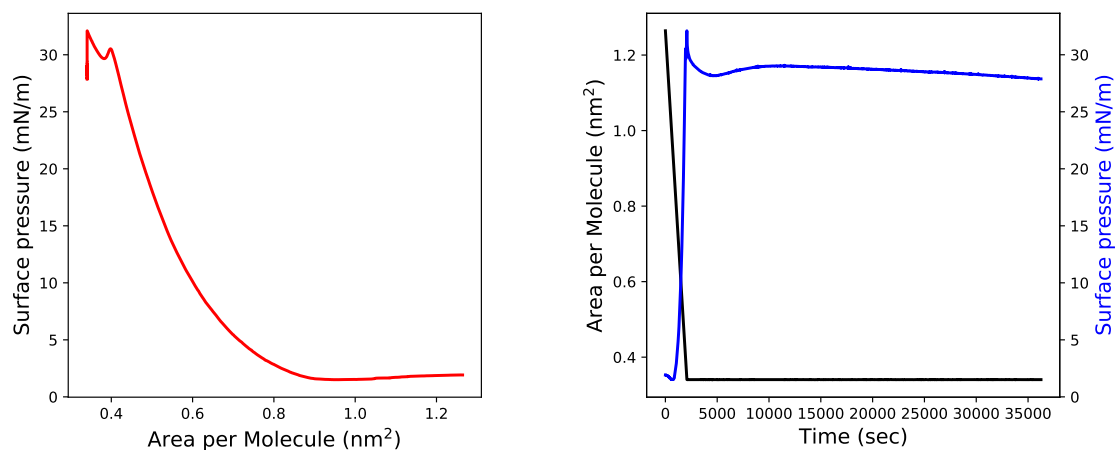
SIRIUS_2020_03_12_0756.nxs

$\pi = 19.74 mN.m^{-1}$

$\gamma = -0.0004715 deg$

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GIXD w/o approx.

$\pi = 19.74 mN. m^{-1}$

$\gamma = -0.0004715 deg$
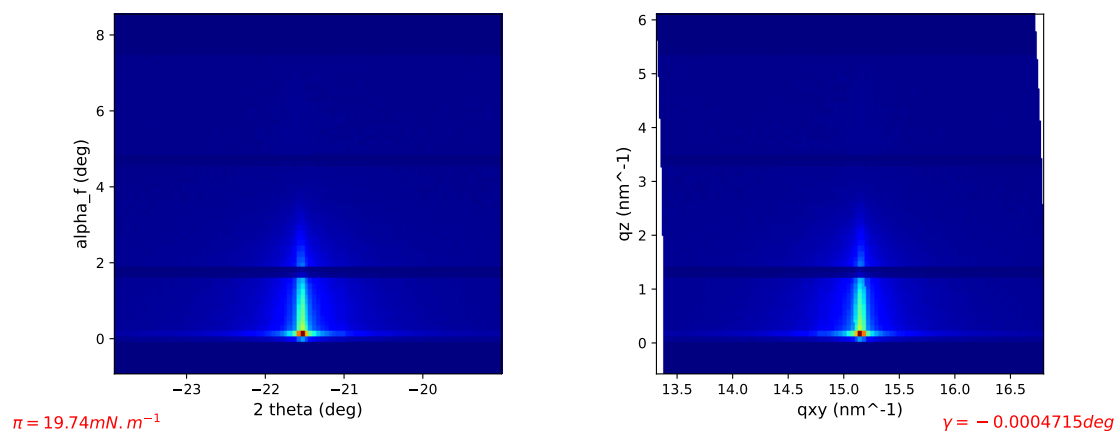
4 Isotherm

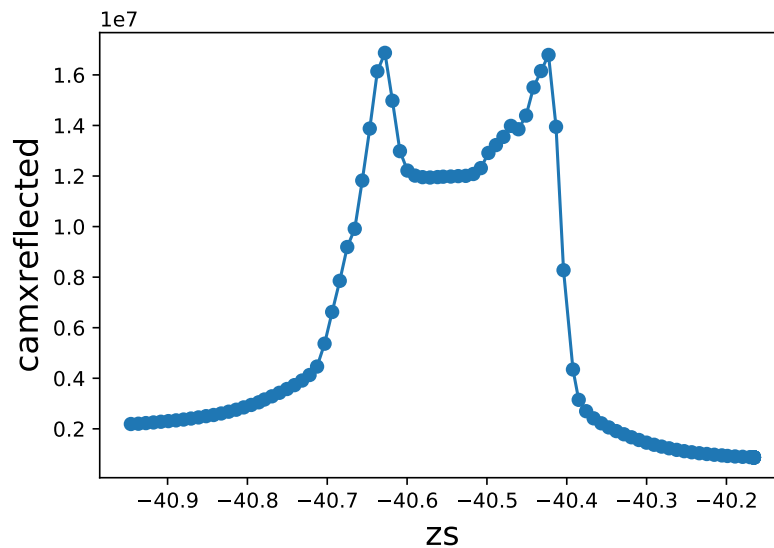### 4.0.1 SIRIUS_Isotherm_2019_02_17_01544: isotherm 1.97 46 35000 1

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
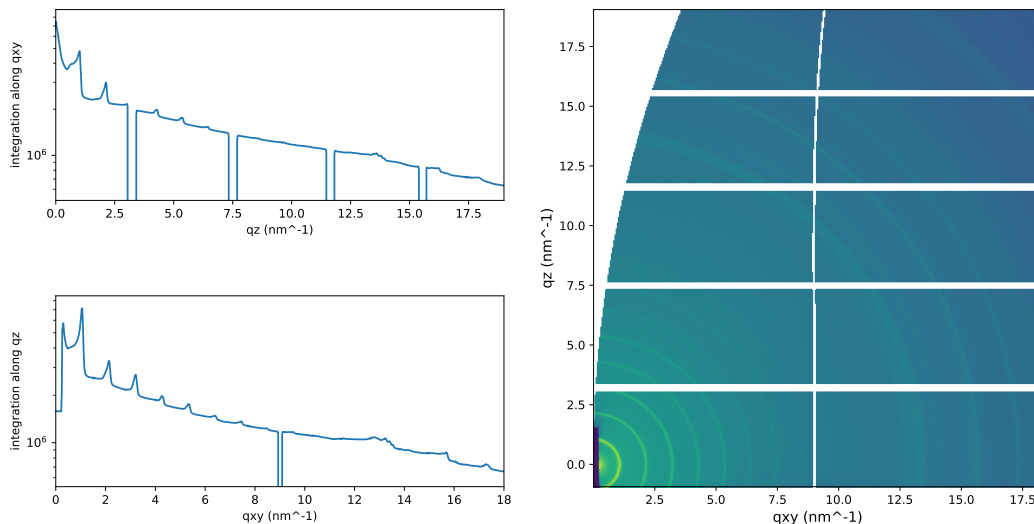
GIXS: q_z vs q_{xy}.

Image with the true geometry, 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

```
. Absorbers: 29 - Vide
. No gamma found! gamma = 0
. No delta found! delta = 11.578
```
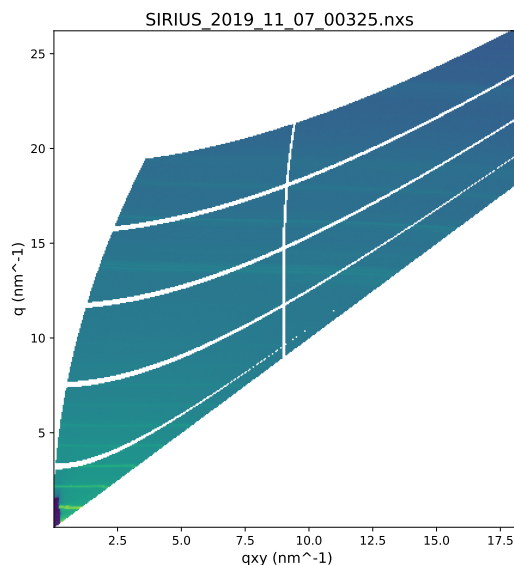
SIRIUS_2019_11_07_00325.nxs

6.0.2 SIRIUS_2019_11_07_00325: tscan 10 10

GIXS: q vs q_{xy}.
Generates:
- SIRIUS_2019_11_07_00325_pilatus_sum.tiff
- SIRIUS_2019_11_07_00325_pilatus_sum.mat

```
    . Absorbers: 29 - Vide
    . No gamma found! gamma = 0
    . No delta found! delta = 11.578
```


SIRIUS_2019_11_07_00325.nxs
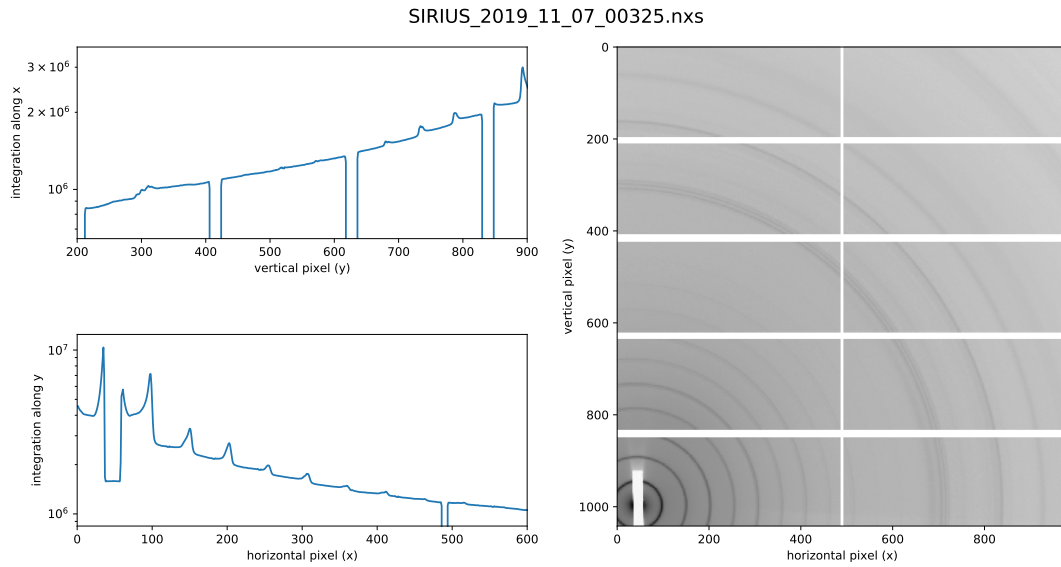
7 Plot pilatus

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
```
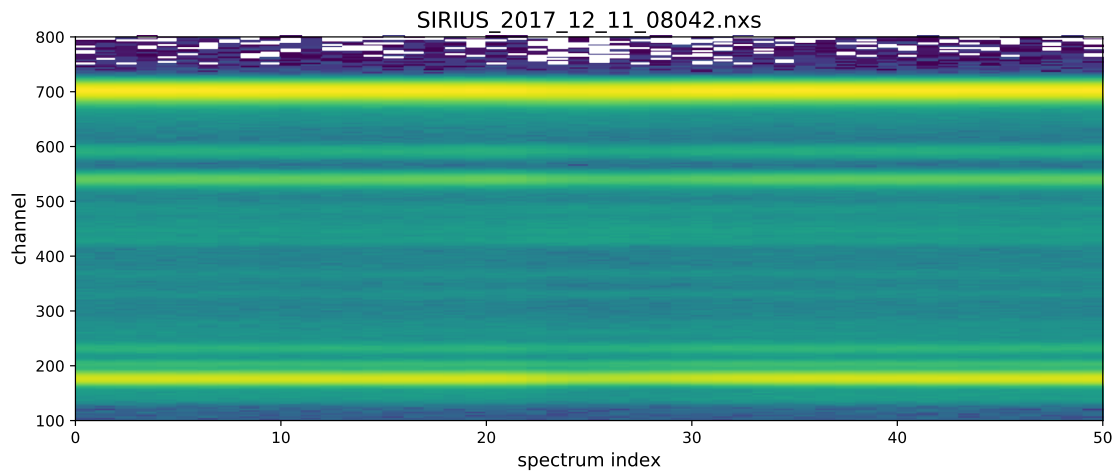
SIRIUS_2019_11_07_00325.nxs

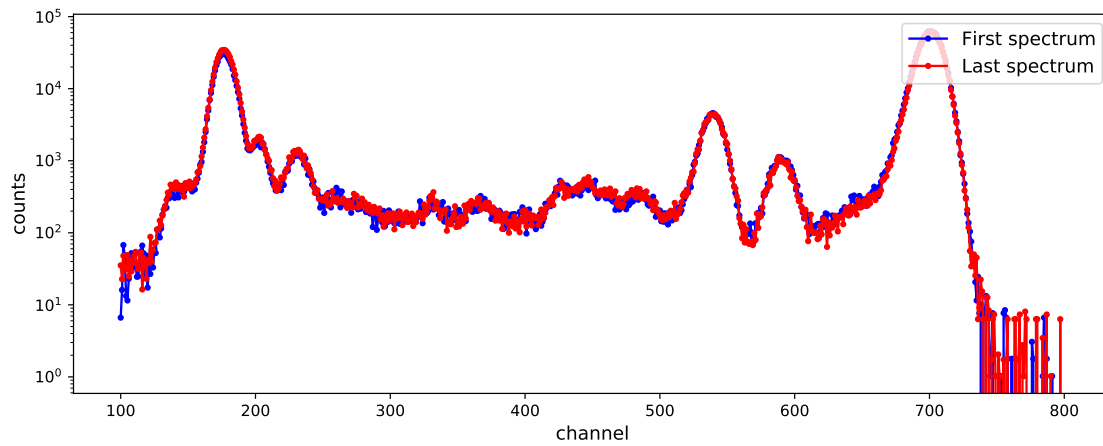# 8 XRF

8.0.1 SIRIUS_2017_12_11_08042: run xsw7.ipy

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
```


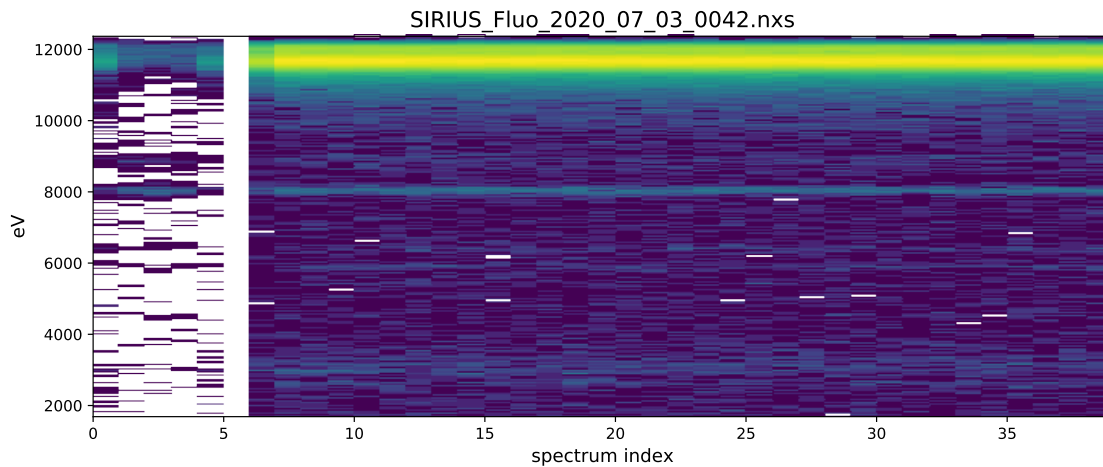SIRIUS_2017_12_11_08042.nxs
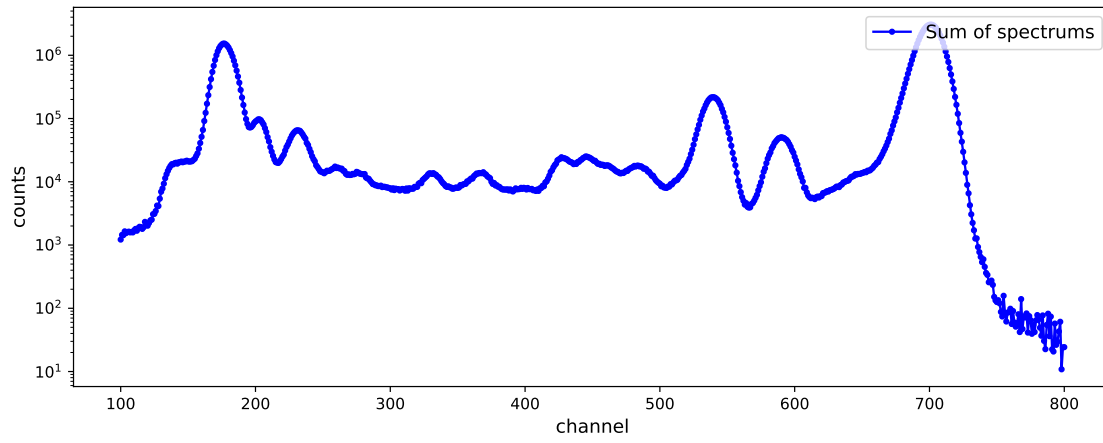
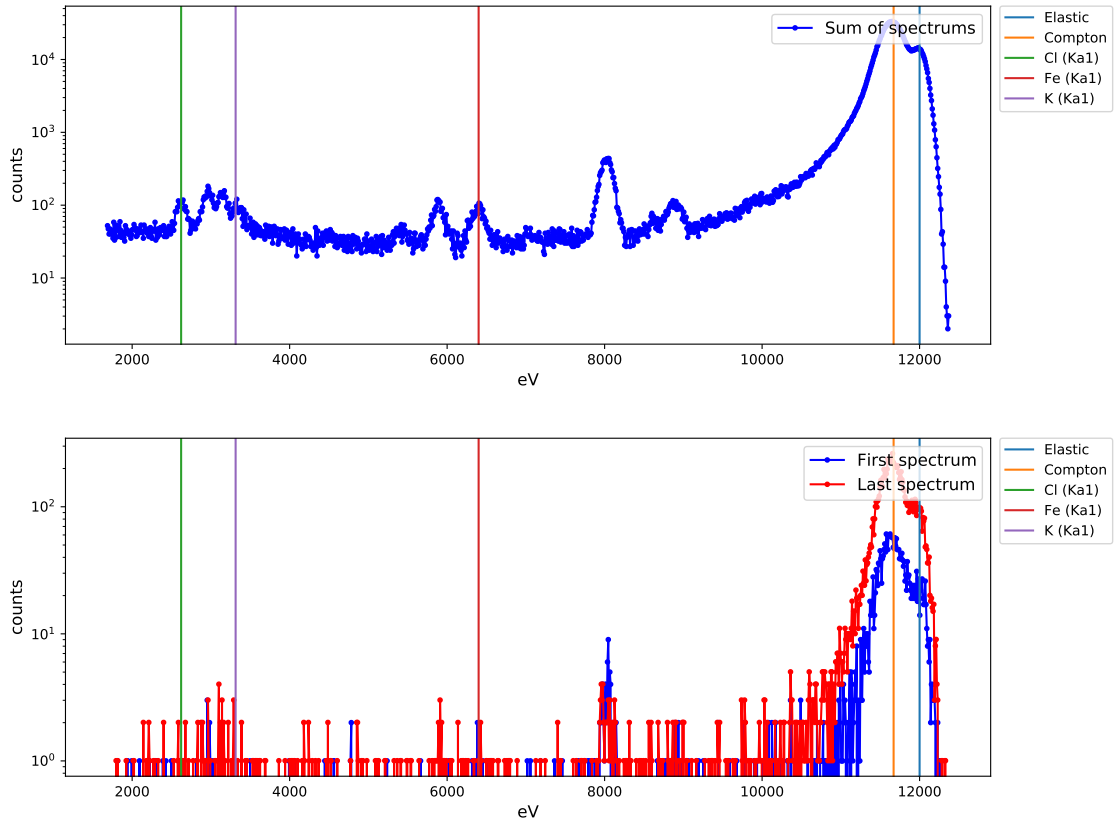## 8.0.2 SIRIUS_Fluo_2020_07_03_0042: tscan 500 30

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

SIRIUS_Fluo_2020_07_03_0042.nxs

9 Insert script

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

9.0.1 script_with_loop.ipy

```
%shopen
%amove delta -40
%run reset_motors.ipy
%amove delta -35
%continuous_ascan delta -35 -25 250 5 #123
%run reset_motors.ipy
for i in range(4):
    %amove delta -20
    %continuous_ascan delta -10 -3 175 5 #124 #126 #128 #130
    %run reset_motors.ipy
    %run cont_regh_abs.ipy #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.ipy
    %run cont_regh_abs.ipy #133 #136 #139
    %run cont_regh_abs.ipy #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
Degrees	1.00196 deg	-89.57961 deg	90.42039 deg	-0.00580	-0.08252

kappa_l	qxy	qxy0	qz	basexPoint	basexTrait
-0.18486	2.0556 nm-1	23.82 nm-1	-0.92 nm-1	-15.7275	-15.7274

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

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

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"'.

11.0.1   List of 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"'.