Swiss-Norwegian
BeamLines

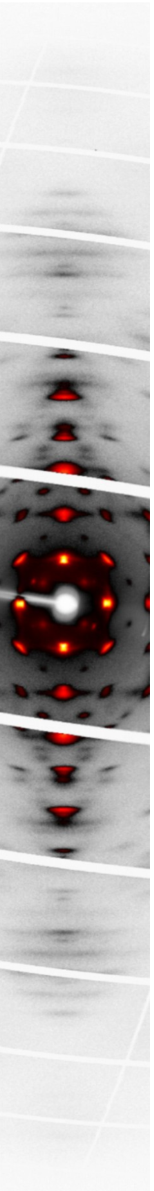
# Bubble@SNBL

Let’s make powder diffraction simple again

# Outlook

- SNBL experiments and users
- In-situ powder diffraction and what users need from us
- Bubble architecture and history
- Additional features
- Future plans for the beamline

# SNBL BM01

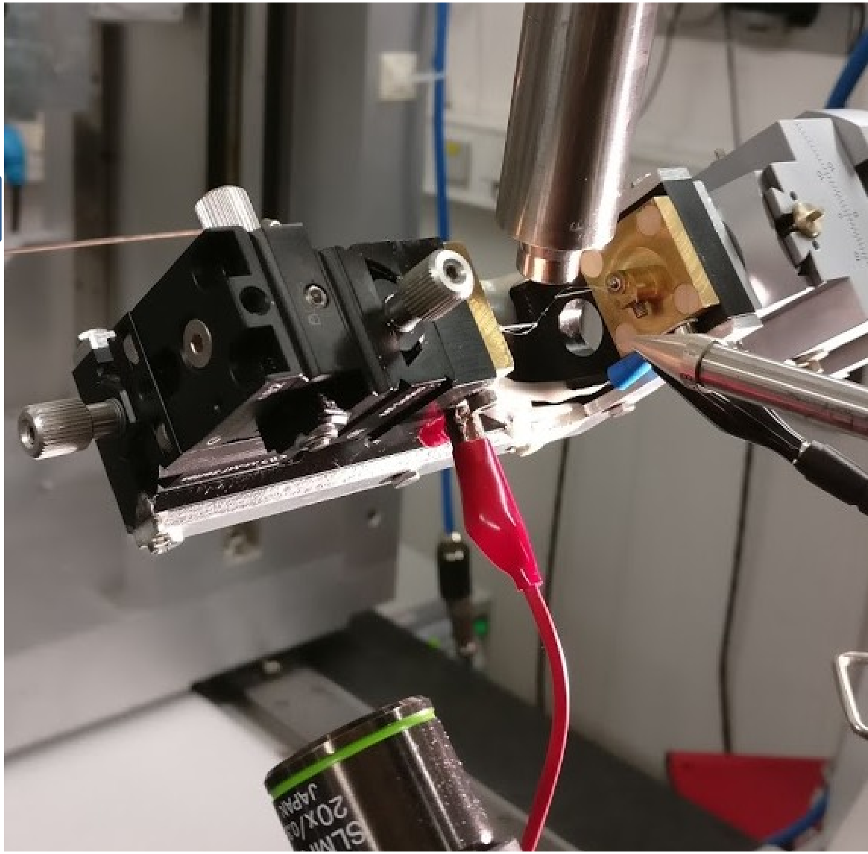


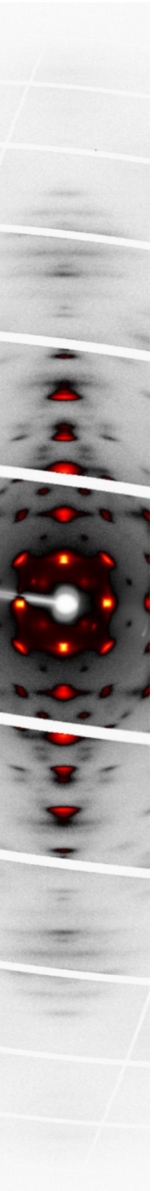
- Small molecule crystallography
- Diffuse scattering
- Powder diffraction/thin films

- A variety of  sample environment tools
- Raman spectrometry, UV-Vis

- Flexible detector positioning
- Flexible kappa goniometry
- Stable optics  with focused beam
- Simple alignment procedures

- Simple and friendly software
- Local data storage
- Data processing tools





Inorganic Chemistry

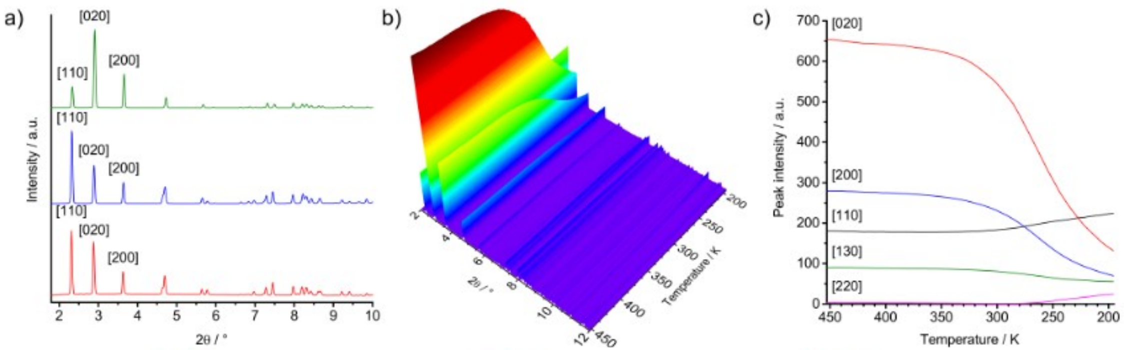
Article

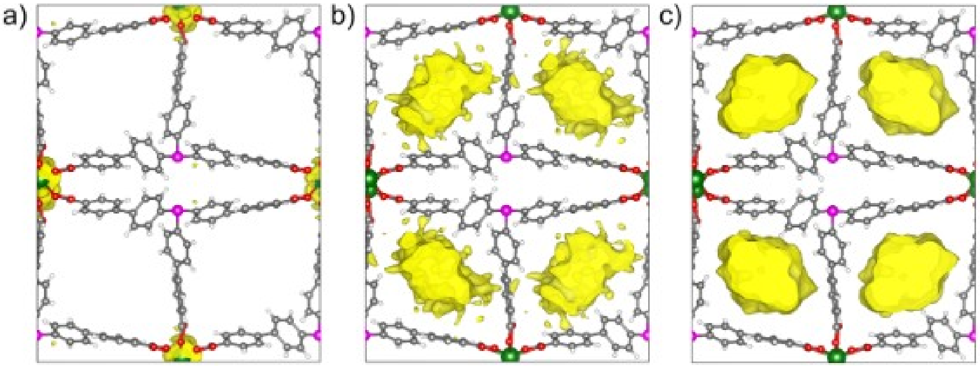
pubs.acs.org/IC

# A Permanently Porous Yttrium−Organic Framework Based on an Extended Tridentate Phosphine Containing Linker

Andrey A. Bezrukov and Pascal D. C. Dietzel*

Department of Chemistry, University of Bergen, P.O. Box 7803, N-5020 Bergen, Norway




- High-intensity or high-resolution modes at one diffractometer
- Large variety of sample environment tools
- Time resolution of 0.1 sec

**An In-Depth Structural Study of the Carbon Dioxide Adsorption Process in the Porous Metal–Organic Frameworks CPO-27-M**

Dr. Breogán Pato-Doldán, Dr. Mali H. Rosnes and Prof. Pascal D. C. Dietzel*

Version of Record online: 16 MAR 2017

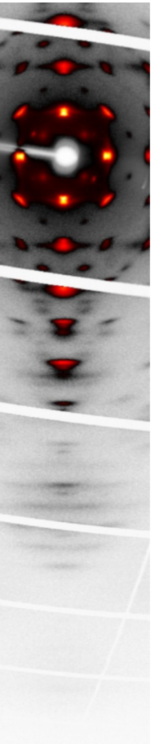
DOI: 10.1002/cssc.201601752

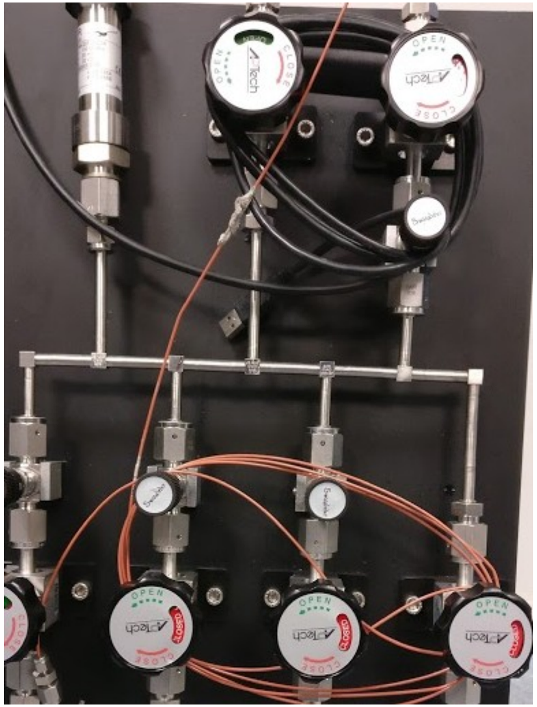


Issue

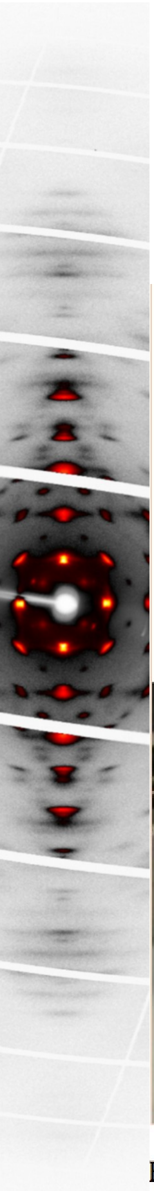

ChemSusChem

Volume 10, Issue 8, pages 1710–1719, April 22, 2017





- Easy programming of complex scenarios and data processing
- In-situ gas loading systems

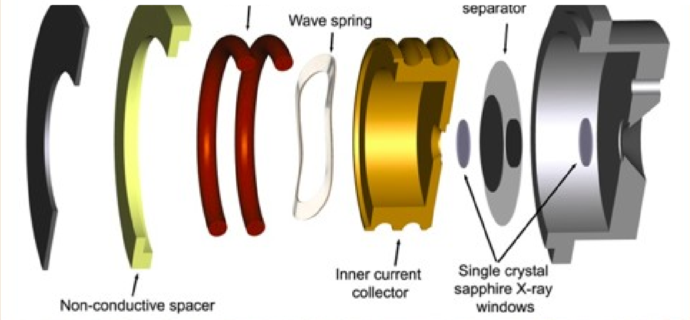


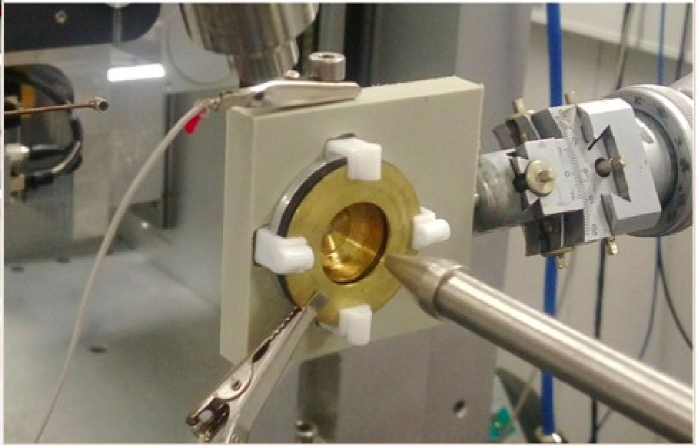
# Electrochemistry in-situ – new Li-battery cell

ARTICLE IN PRESS – J. Synchrotron Rad.

JSR JOURNAL OF SYNCHROTRON RADIATION
ISSN 1600-5775

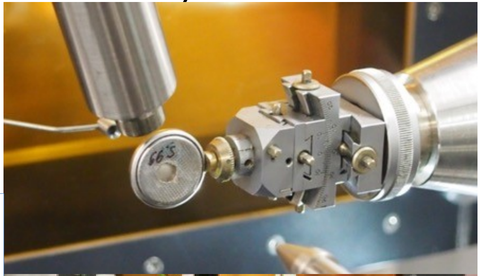
**An electrochemical cell with sapphire windows for *operando* synchrotron X-ray powder diffraction and spectroscopy studies of high-power and high-voltage electrodes for metal-ion batteries**

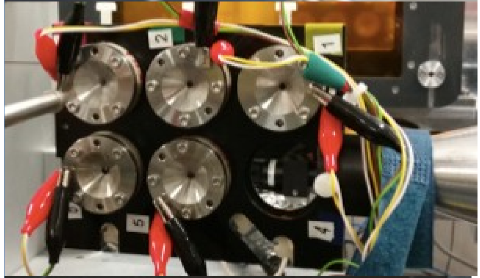


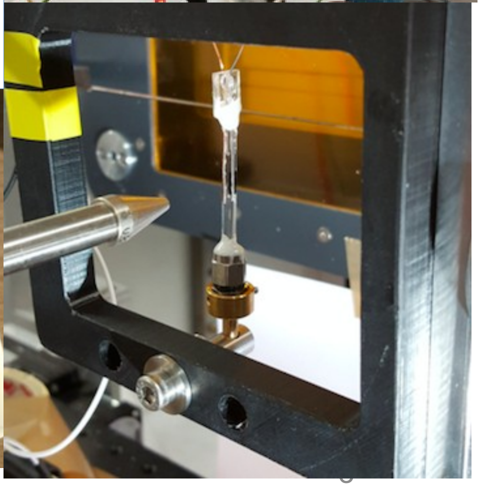



Exploded view and photo of the novel *operando* electrochemical cell.

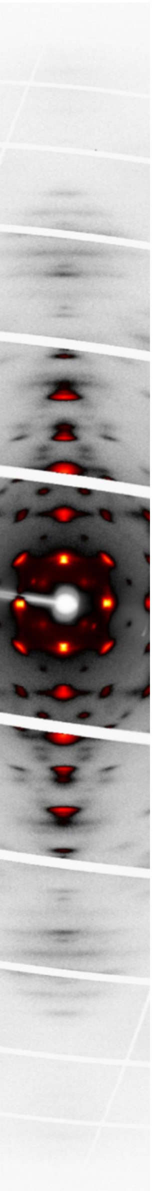
- Inspired by users experiments
- Compatible with two BLs
- Professional design, lab-tested
- Na-battery will be soon

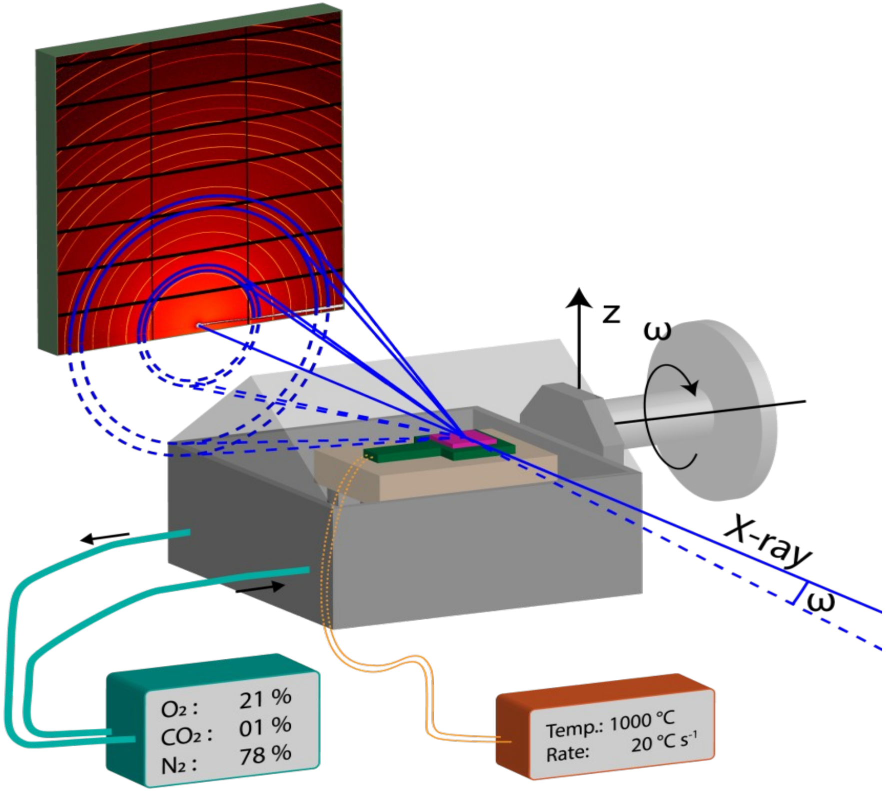


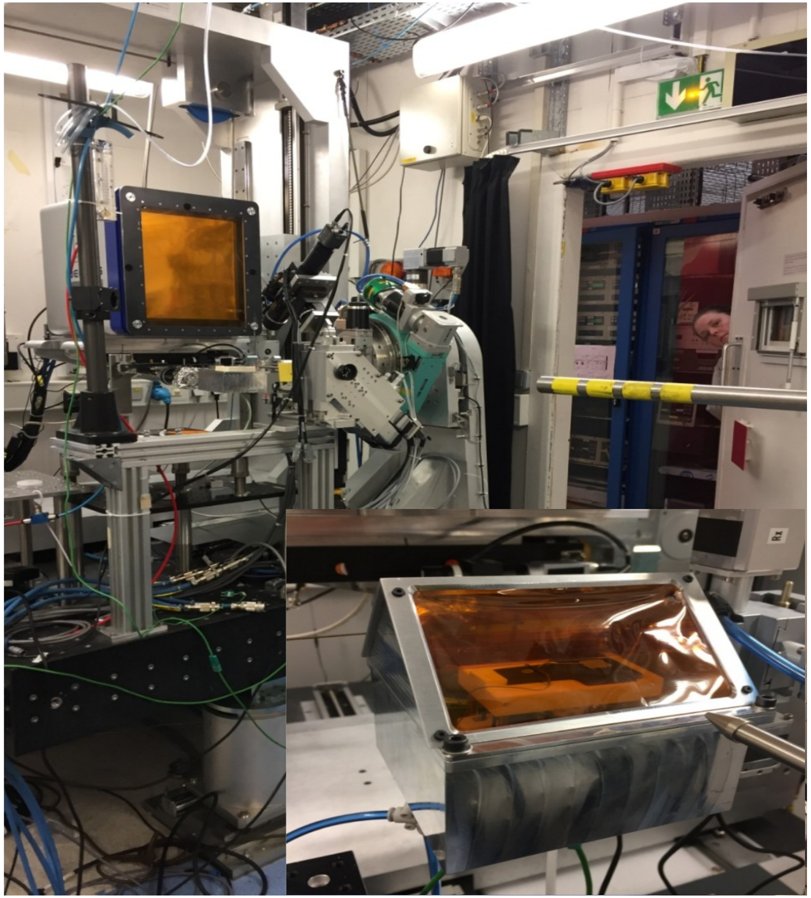




# In-situ thin film processing





# What users need from us

1. We have a variety of user expertise and experience, from master students to professors from food industry to fundamental physics
2. In situ experimentation needs an on-line inspection of the results in order to optimize or alter experimental strategies
3. The measured data have to be processed just after the data collection in a form that is close as possible to results

Year 2017 BM01 gave more than 75 publications
Year 2018 BM01 gave more than 80 publications

# Bubble@SNBL

Is Bubble an alternative GUI for pyFAI?

- Hmm, probably not… I would call it pyFAI-on-steroids.

Is Bubble going to integrate my data from @XYZ@ beamline?

- It may, but most likely not…

Why?

- Because Bubble is not a universal program for everyone (like Fit2D, pyFAI-calib2 or Dioptas).
- Bubble is the specialized beamline software to make life easier for beamline scientists and beamline users.
- Bubble is optimized for certain beamlines and certain measurement strategies. If your data are not measured on those beamlines using those strategies, Bubble may not work for you. Those beamlines are: SNBL (BM01, BM31), Dubble (BM26), BM20 (ROBL), ID28, ID11 (to a certain extent). The list is yet to be extended.

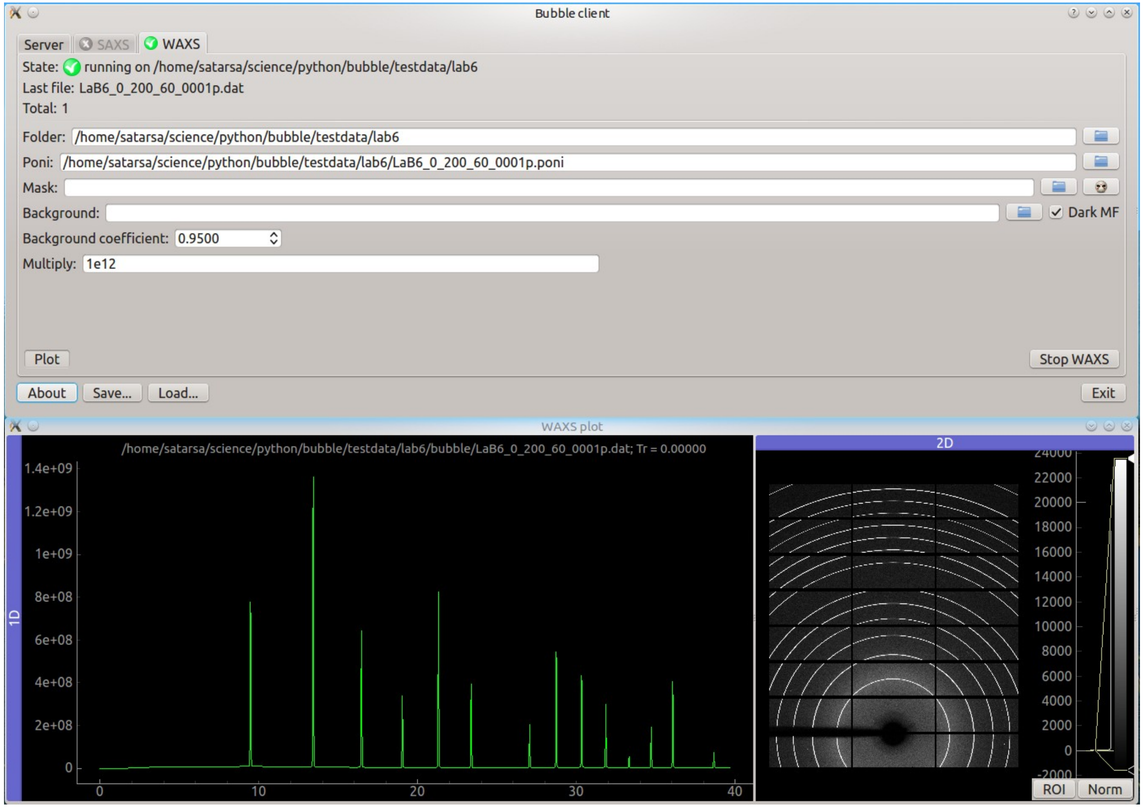
# Bubble history

Bubble started as a tool to simplify SAXS and WAXS integration on the Dubble beamline

Before:

```
# For calibration only
0) /scisoft/bin/pyFAI-calib -pix=172e-6,172e-6 filename

# For data reduction
1)ssh connection to user account

ssh -X userid@rnice
type password

2)go to bm26 directory
cd bm26

3)edit info file (if not open already)
nedit par_SAXS_WAXS.info &

4)start matlab
matlab -nodesktop

5)add path in matlab
addpath('~portale/pyfai2')

6)run macro
pyFAI_data_reduce_edf_series('par_SAXS_WAXS.info','SAXS','filename1_SAXS','filena

or

pyFAI_data_reduce_edf_folder('par_SAXS_WAXS.info')


If an error appears and the connection to rnice is reset then do the following.
1)ssh connection to user account

ssh -X userid@rnice
type password

2) Go to home directory
cd ~

3) remove the temporary matlab folder (this will delete the matlab command
history)
rm -rf .matlab
```

After:

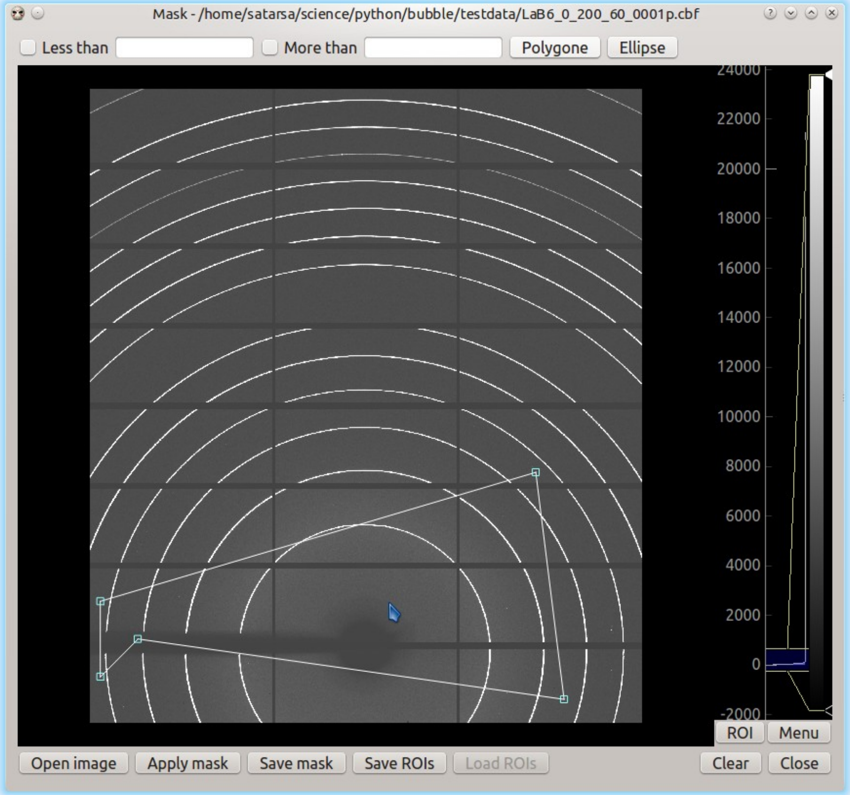


# Integration algorithms

Server uses bounding box pixel splitting. No other choices are possible. Calibration is done via pyFAI-calib.

Features:

- On-line integration.
- Masking.
- Azimuthal and radial borders.
- Background subtraction.
- Normalization on the monitor counts, median and sum values, background
- Dark current, geometrical distortions for CCD detectors.
- Calculation of the sample transmission for SAXS data, taking into account thickness and concentration of sample.

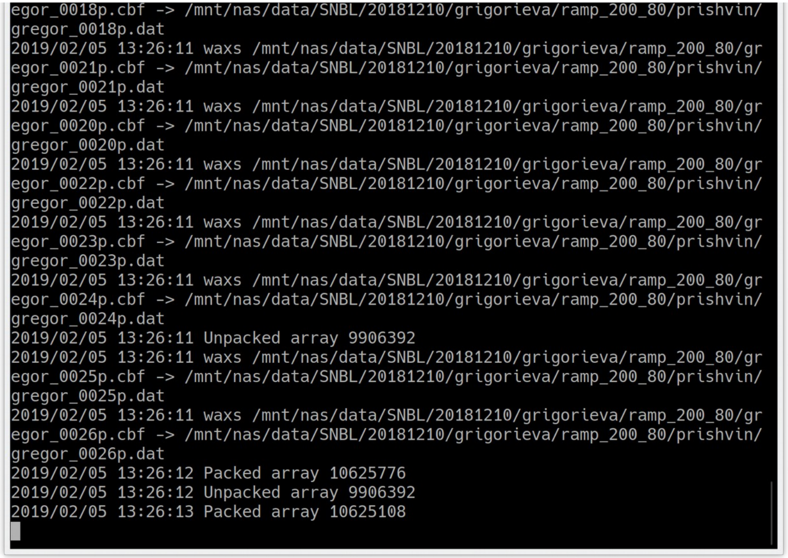


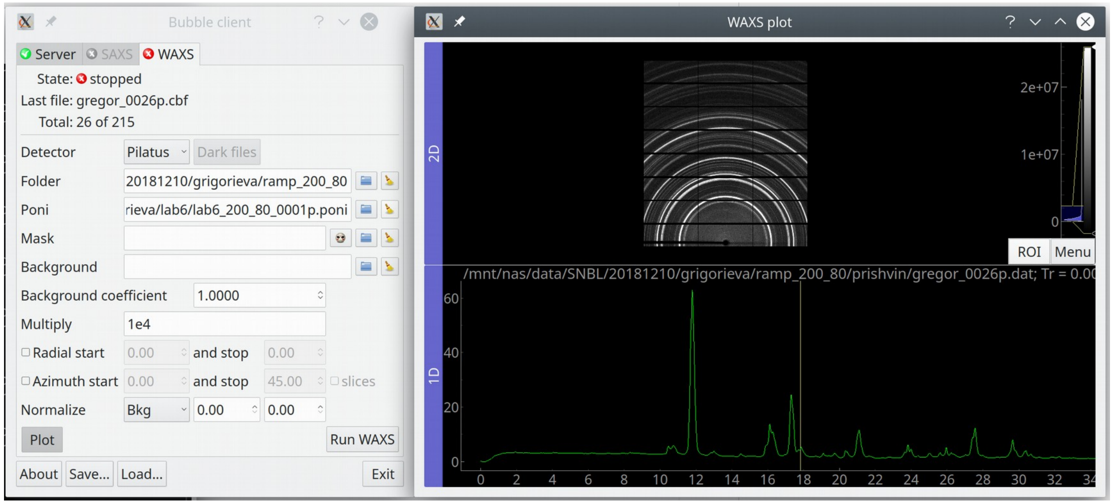
# Bubble architecture, version 1 (2014-2015)

## Client-server architecture

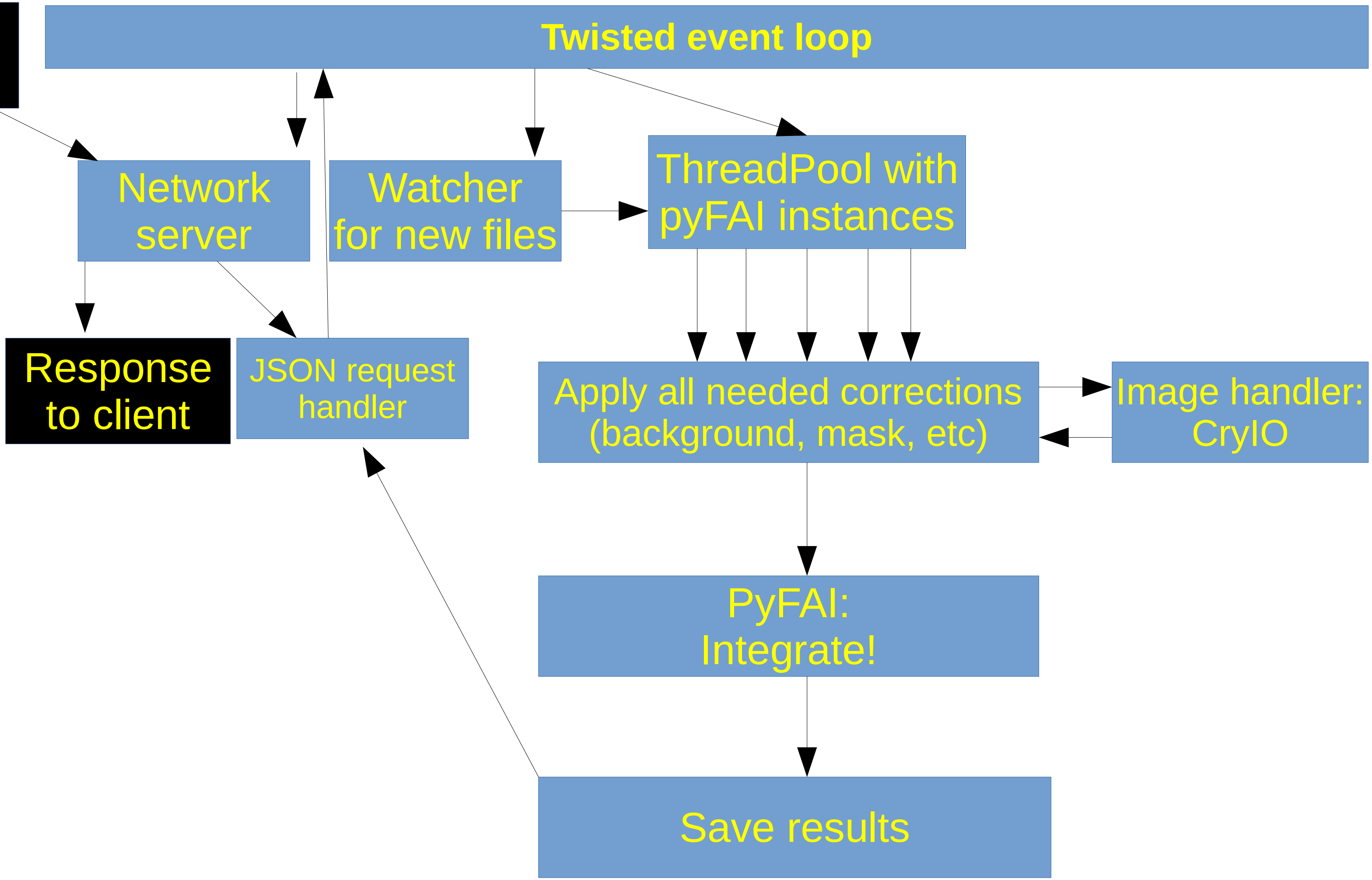
Server: cross-platform Python2 CLI application, using Twisted, asynchronous network framework.

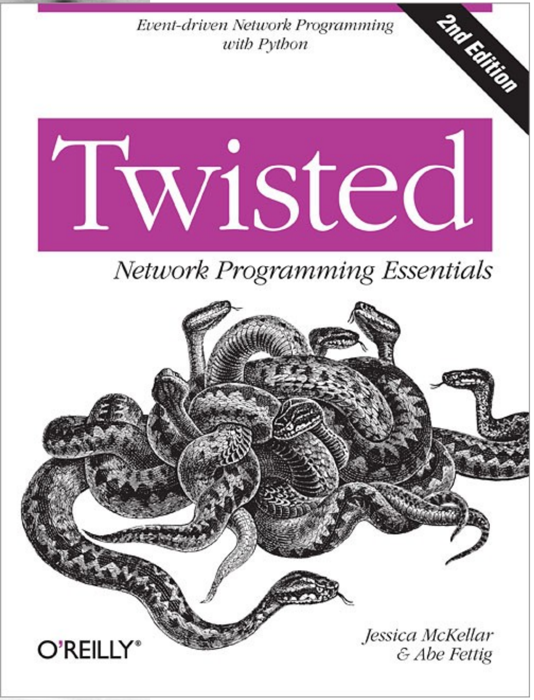
Client: cross-platform Python2 application, using PyQt4 GUI framework.



# Bubble architecture, version 1

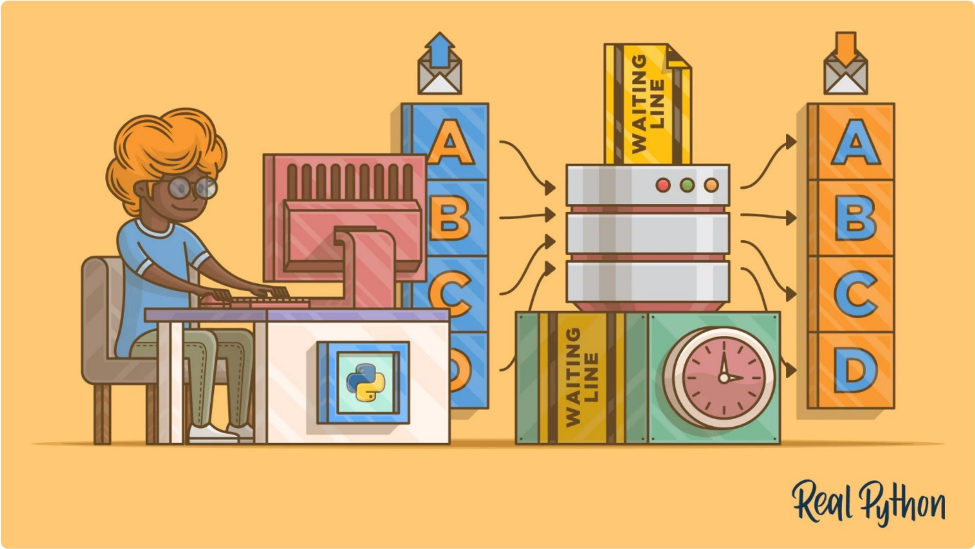


# Bubble architecture, version 2 (2015-2018)

Still the same client-server architecture, but:

- Server: cross-platform Python3 CLI application, using AsyncIO, asynchronous framework.
- Client: cross-platform Python3 application, using PyQt5 GUI framework.




**Async IO in Python: A Complete Walkthrough**

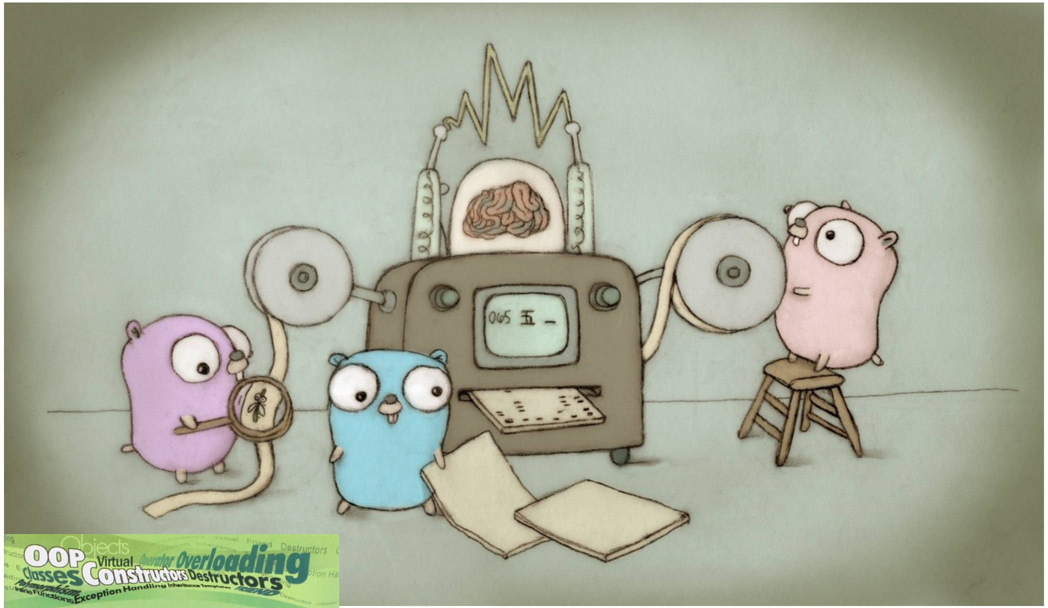
# Fundamental Python limitations

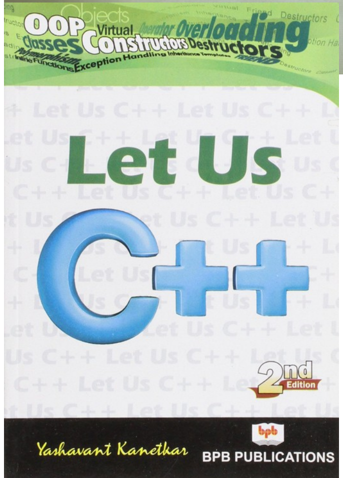
- GIL – Global Interpreter Lock, you can run only one thread at a time, but you do still have all the pleasure of multi-threading programs: race conditions, deadlocks, starvation, etc. Workarounds are difficult:
  - pure C-extensions with macros **Py_BEGIN_ALLOW_THREADS** and **Py_END_ALLOW_THREADS**
  - Cython extensions ‘**with nogil**:’
- At some point pyFAI started to use thread locks which blocked the asyncio event loop, resulting in random deadlocks.
- pyFAI became very thick, some GUI parts appeared in the code base and they unconditionally imported PyQt. The final executable of the Bubble server after ‘pyinstaller’ was about 500 Mb, it pulled the whole PyQt framework as a dependency, not even using it.

# Bubble architecture, version 3 (since 2018)

Still the same client-server architecture, but:

- Server: cross-platform CLI application, written from scratch in the Go programming language.
- Client: cross-platform C++ application, using Qt5(6) GUI framework (in progress).





# Bubble architecture, version 3 (since 2018)

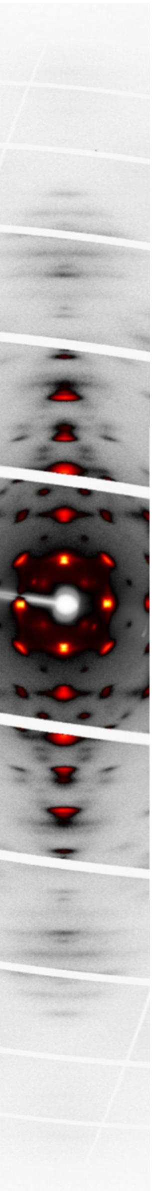

The best from the both worlds of C and Python:

- **Like in C:**
  - Compiles into native code (no JIT, no virtual machines)
  - Everything passed by copy + pointers
- **Like in Python:**
  - Very comprehensive standard library + a lot of 3rd party libraries
  - A lot of embedded objects: strings, slices (lists), maps (dicts), closures, etc
  - Garbage collector, no manual memory handling

- **Unlike both:**
  - No GIL, native light threads, channel for communications between them
  - Very strong static type system + error is a value.
  - The easiest cross-platform compilation ever, in linux just:

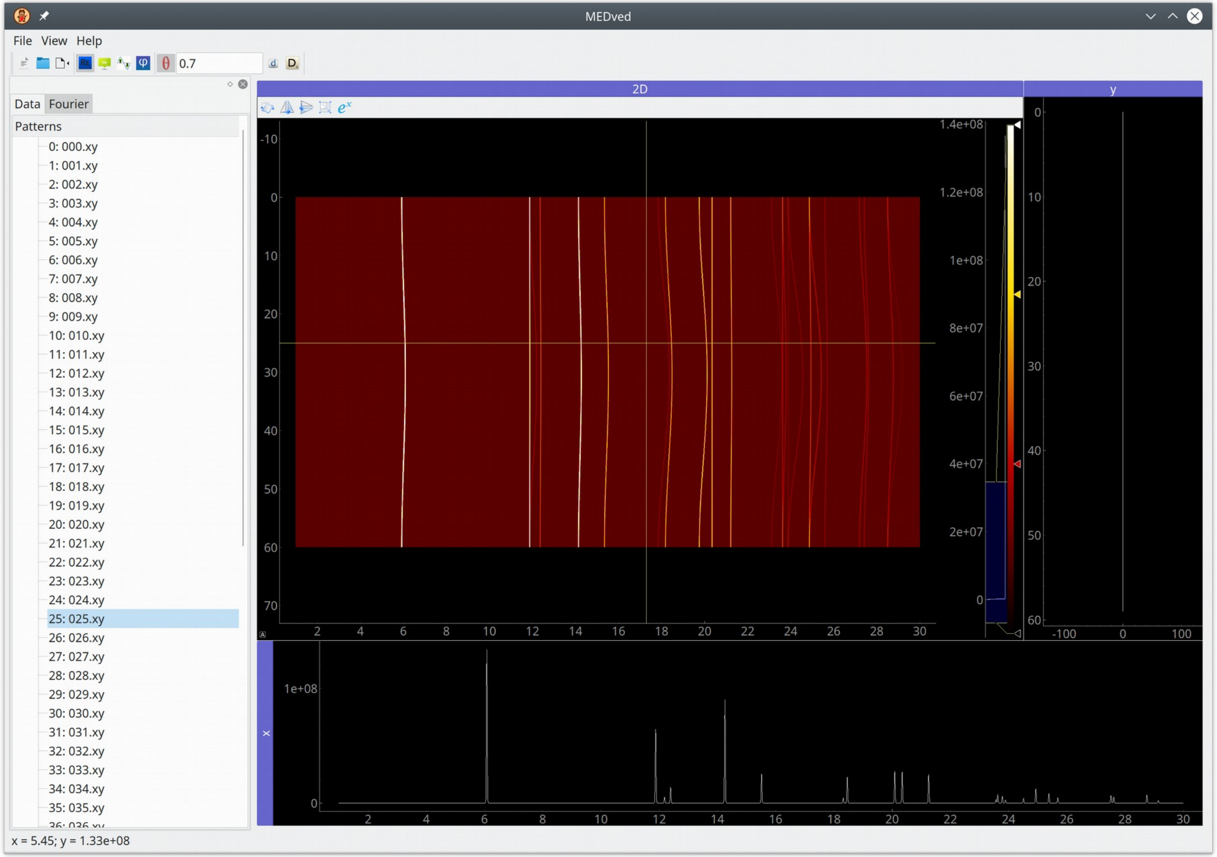
```
$ GOOS=windows go build
```

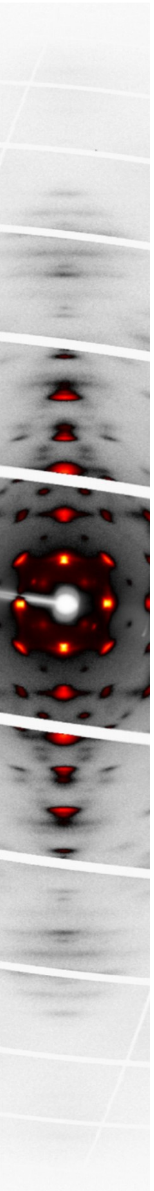
  - Statically linked executables with very moderated size. Deployment becomes a pleasure!



# After integration: MEDVED

A program for the new diffraction method MED: Modulation-Enhanced Diffraction Viewer and Editor. It can be  used to quickly investigate evolution of powder patterns.



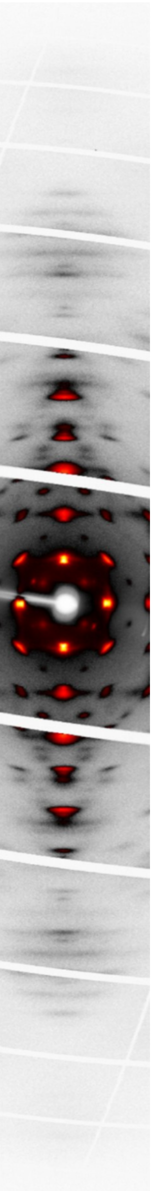


# Download and install

Download: https://soft.snbl.eu/bubble.html

Server source code: https://hg.3lp.cx/bubbleg

Client source code: https://hg.3lp.cx/bubble

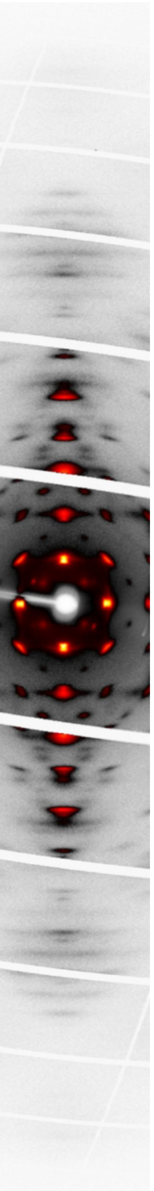


# BM01 to meet future challenges

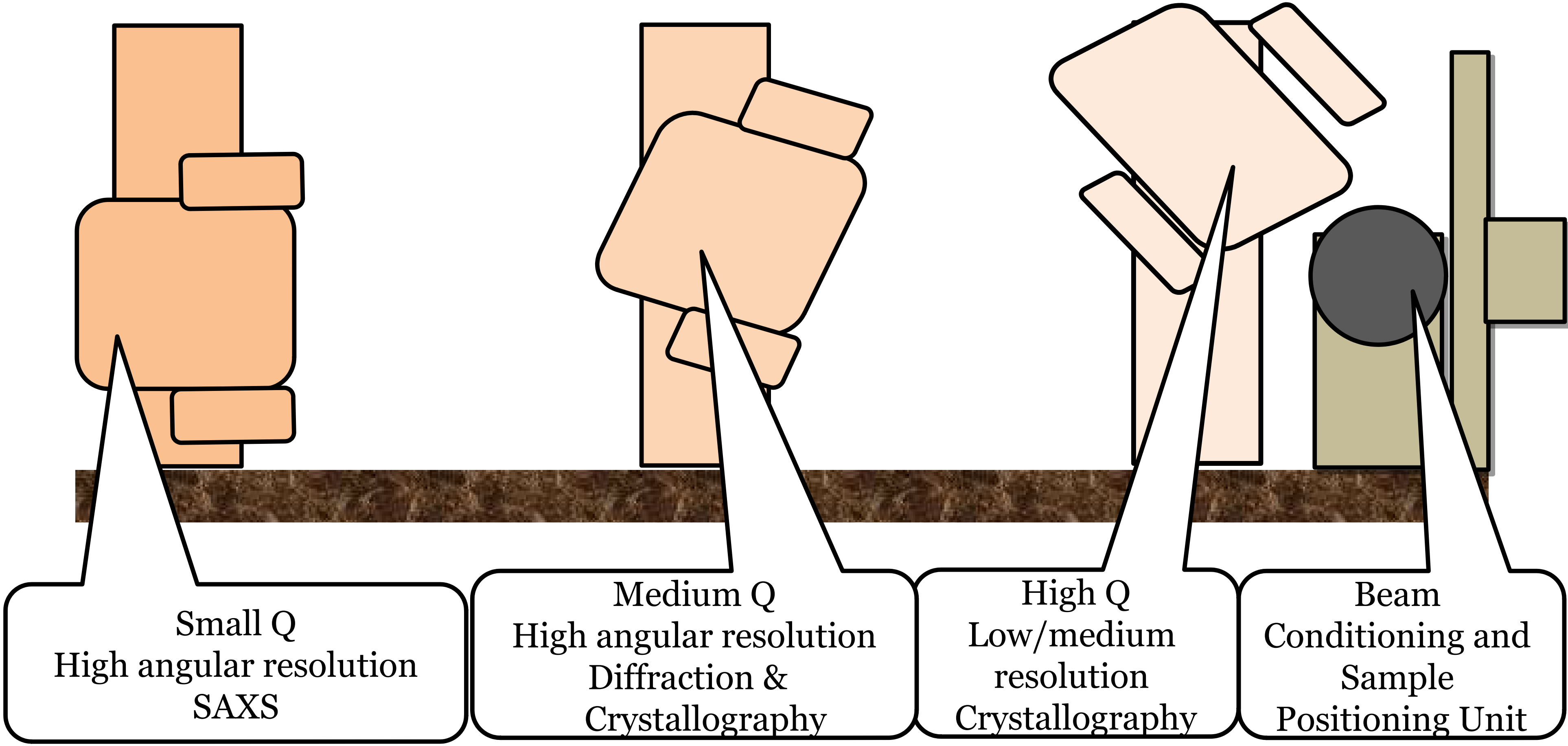
- A combination of diffraction tools at one beamline:
- **Single Crystal diffraction + Powder Diffraction + Thin film diffraction + Small angle scattering**

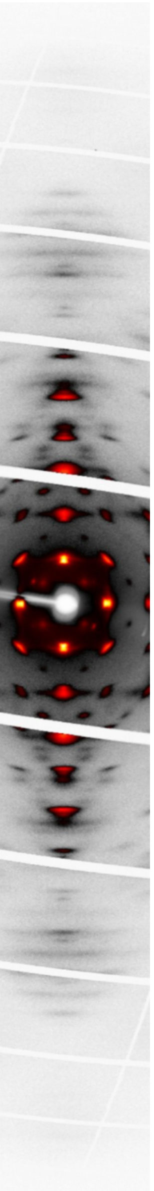
- **Crystallography**: from structure solution to charge density
- **Diffraction**: from dynamic scattering to reciprocal space mapping.

- **Microns / milliseconds resolution for all scattering tools.**



# A concept of the end station





# Charge-density high Q configuration

$$Q_{max} = 4\pi \frac{\sin(\Theta)}{\lambda}$$

Charge density limit.

$$\frac{\sin(\Theta)}{\lambda} \geq 1$$

$$\frac{\sin(40^0)}{0.6} = 1.07$$

$$Q_{max} \equiv 13.46 A^{-1}$$

Expected crystallographic resolution for tilted detector at 20.7 keV

At 22.5 keV such a setup would offer very good charge density data (1.17)

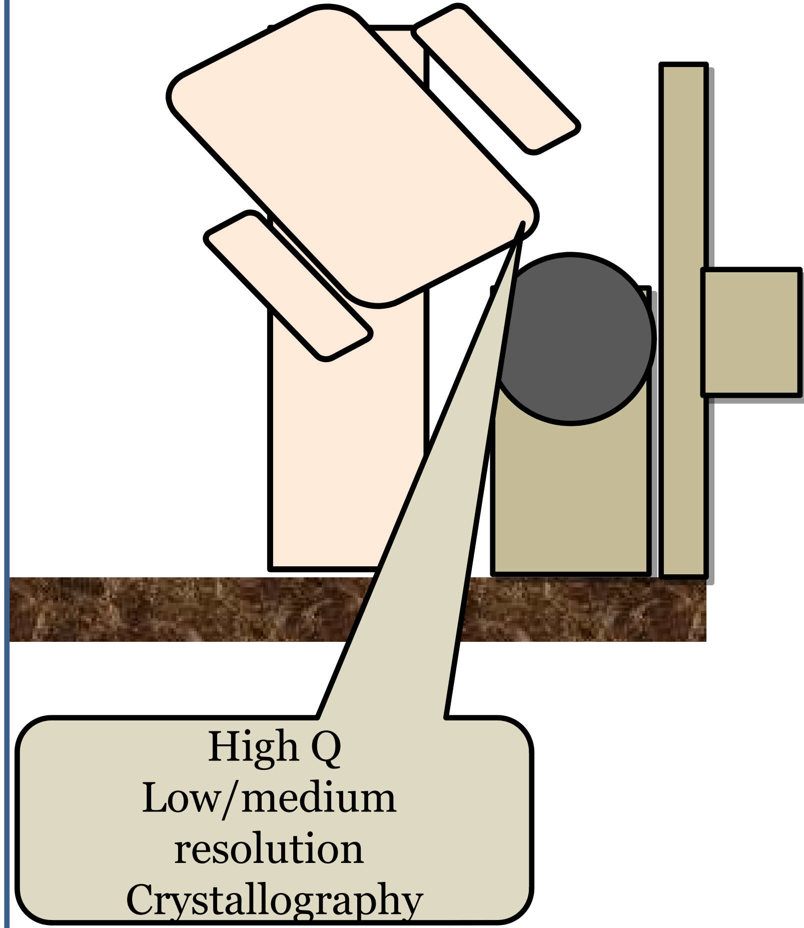
REVIEW

**Concerning the measurement of charge density X-ray diffraction data at synchrotron sources: challenges and opportunities**

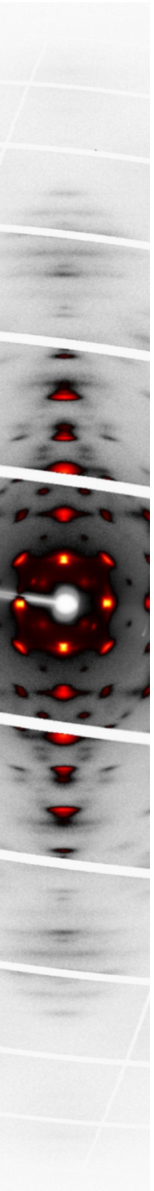
John R. Helliwell

Pages 1-14 | Received 06 Dec 2016, Accepted 09 Feb 2017, Published online: 13 Mar 2017

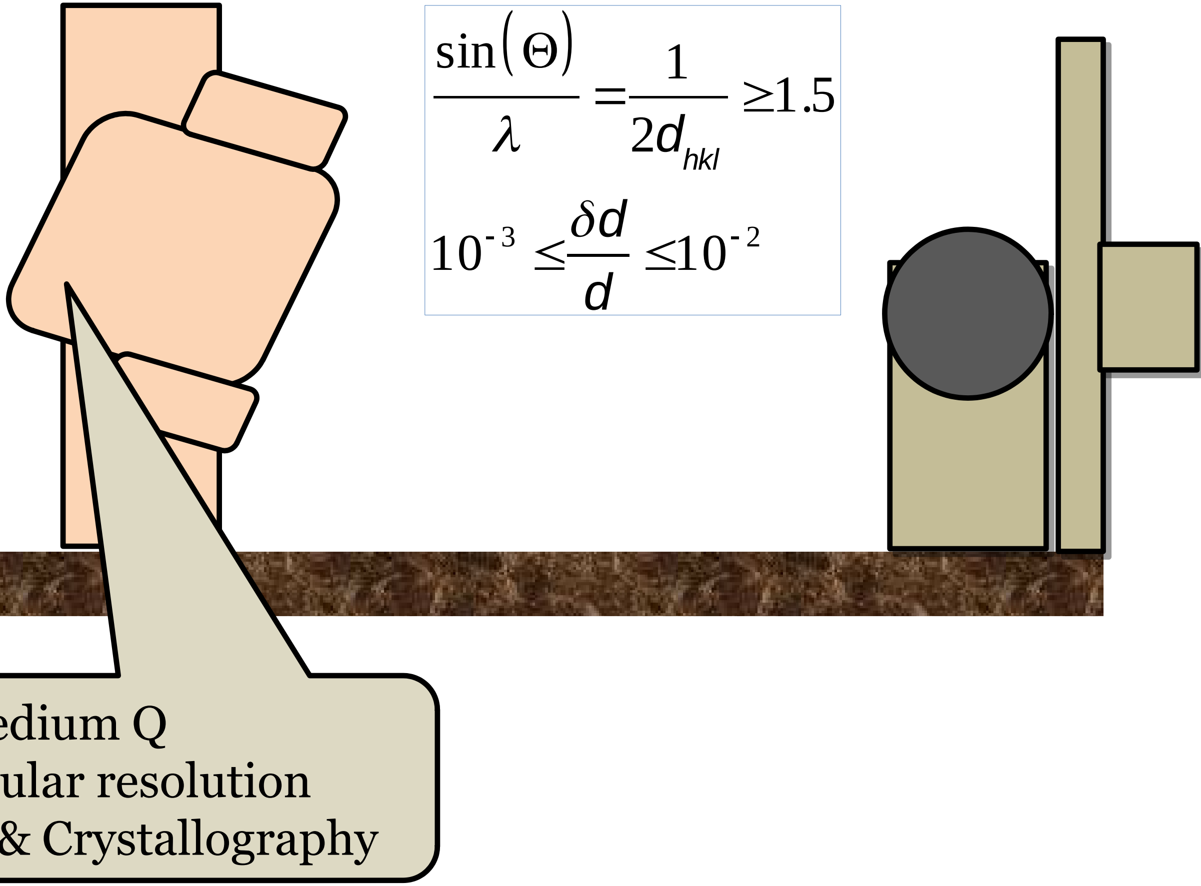
Download citation http://dx.doi.org/10.1080/0889311X.2017.1295038 Check for updates



# Crystal structure determination and analysis



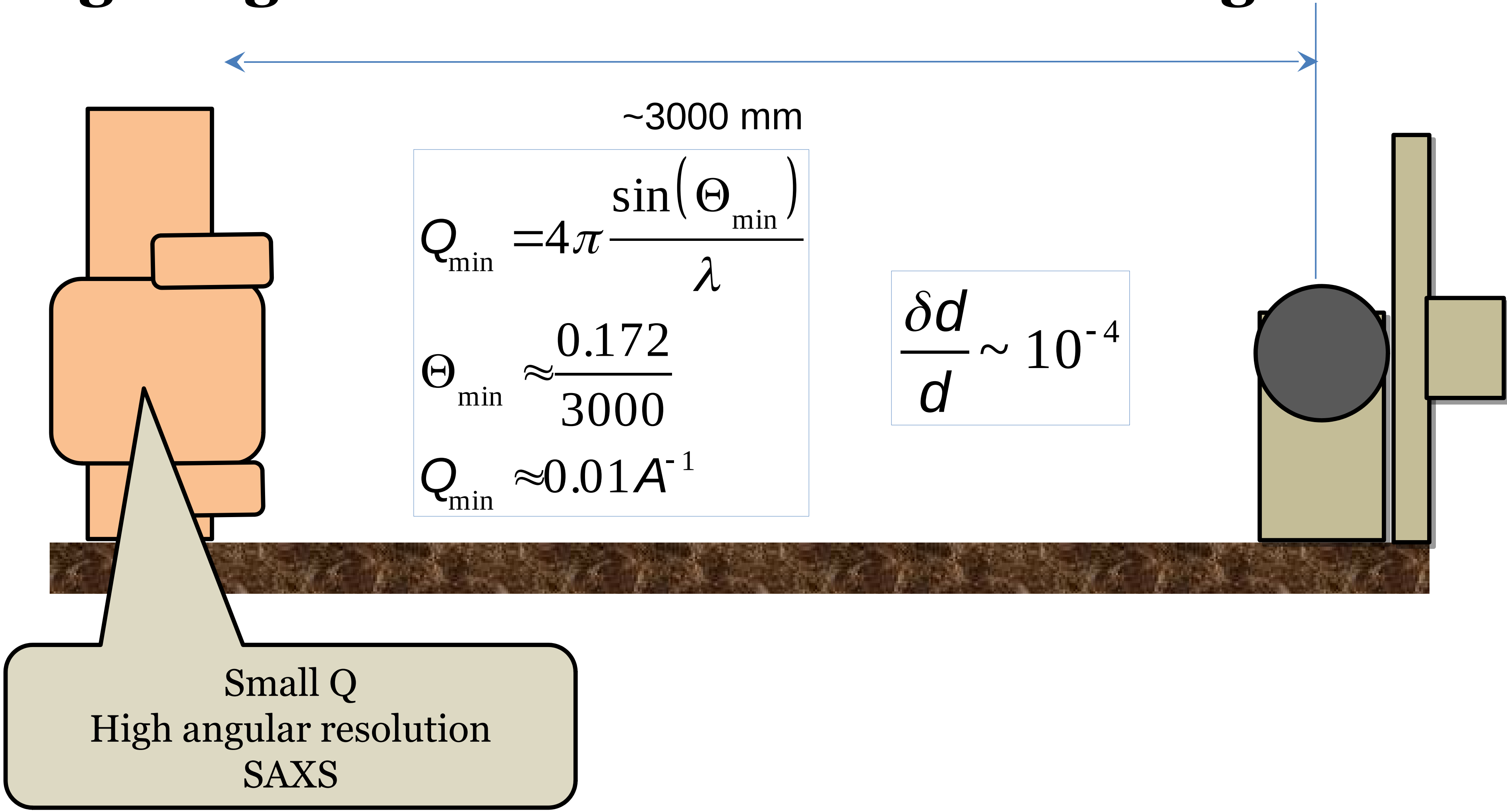
Powder diffraction
Single crystal diffraction
for materials with large unit cells, thin films, diffuse scattering
time resolved diffraction, kinetics, phase transition phenomena




$$\frac{\sin(\Theta)}{\lambda} = \frac{1}{2d_{hkl}} \geq 1.5$$

$$10^{-3} \leq \frac{\delta d}{d} \leq 10^{-2}$$

# High angular resolution and SAXS configuration

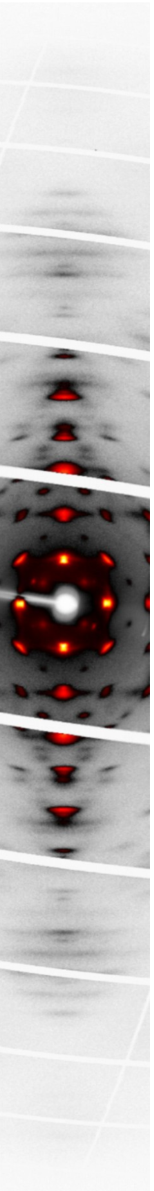



$$Q_{min} = 4\pi \frac{\sin(\Theta_{min})}{\lambda}$$

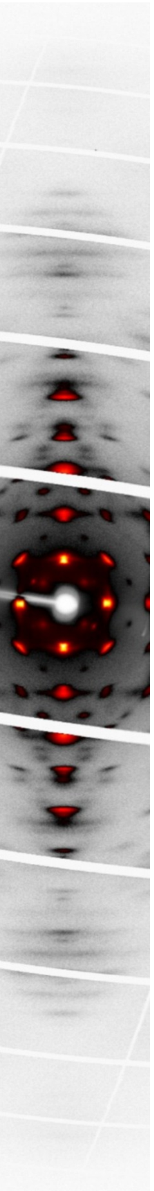
$$\Theta_{min} \approx \frac{0.172}{3000}$$

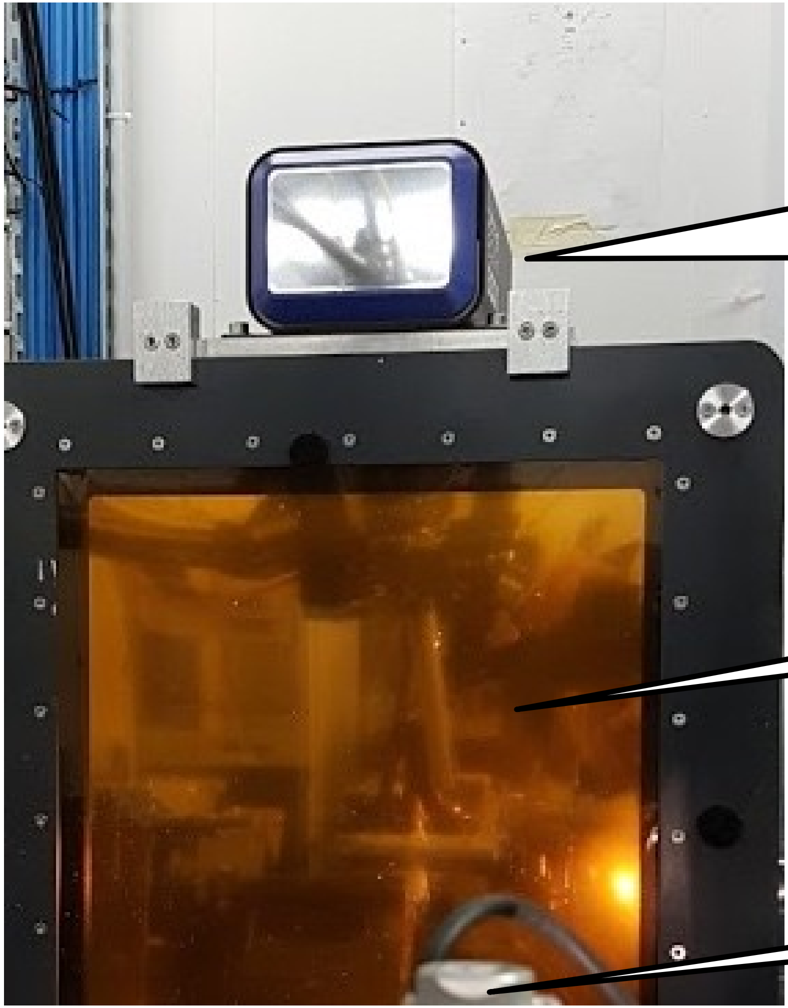
$$Q_{min} \approx 0.01 A^{-1}$$

$$\frac{\delta d}{d} \sim 10^{-4}$$



# Detector Set  for all seasons

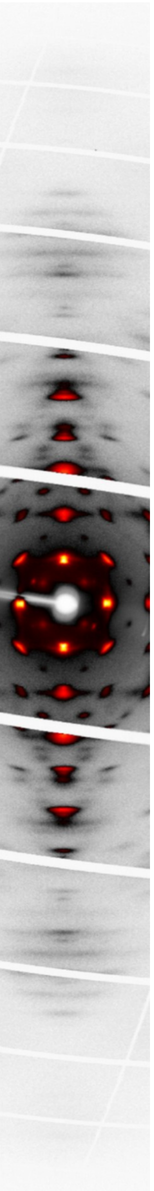




Eiger 500K +
75 micron pixel
Up to 9 kHz readout
For fast data acquisition, local reciprocal maps, and SAXS.

Pilatis 2M
172 micron pixel
30 Hz readout
For wide angle diffraction and crystallography.

Small pixel CCDs for beam alignment and SAXS



# Summary

1. BM01 fills the growing gap between home laboratories and specialized synchrotron beamlines.
2. We combine different diffraction and crystallography tools + wide range of sample environment options.
3. Stable and easy in use beamline + solutions for the data processing, data analysis, data transfer and data storage.

**We want to keep and develop further these options**

4. The range of diffraction tools, covered scattering angles and angular resolutions to be expanded from a charge-density single crystals diffraction to SAXS.
5. With improved beam and new detector system - time resolved diffraction up to $10^{-3}$ s.