# State of the azimuthal integration at the ESRF. Pathway to pyFAI2

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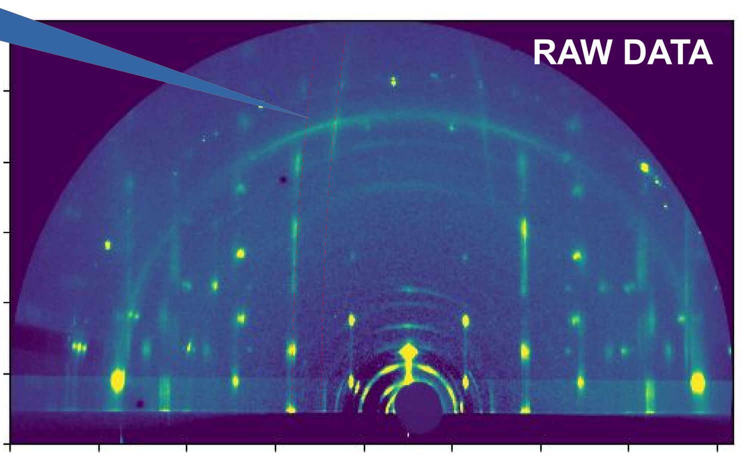
**PyFAI is the standard tool for performing azimuthal integration and data reduction for scattering experiment. Recent enhancements are presented here like the support for grazing incidence / surface diffraction, the diffraction-map visualizer, the support for detector flipping and the signal separation based on sigma-clipping which enables lossy compression and peak-finding for single crystal experiments.**

## *Grazing-Incidence / Fiber diffraction support*

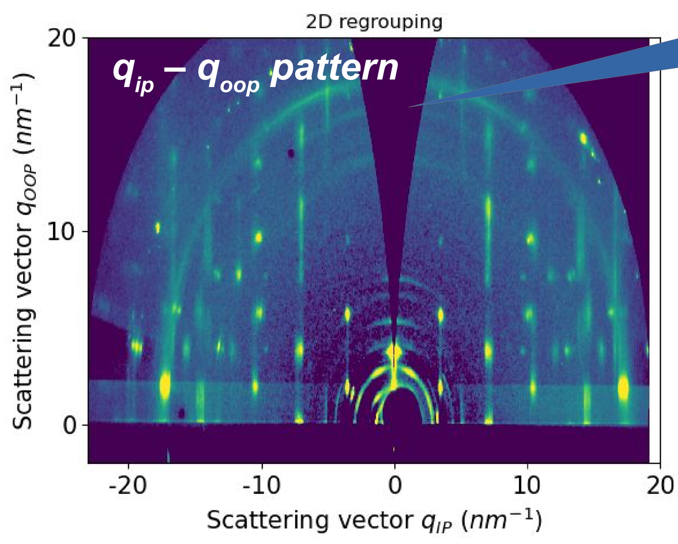
In a flat detector, the diffraction rods are curved




***Reshaping into the components of the*** $\vec{q}$ ***(momentum transfer) vector***

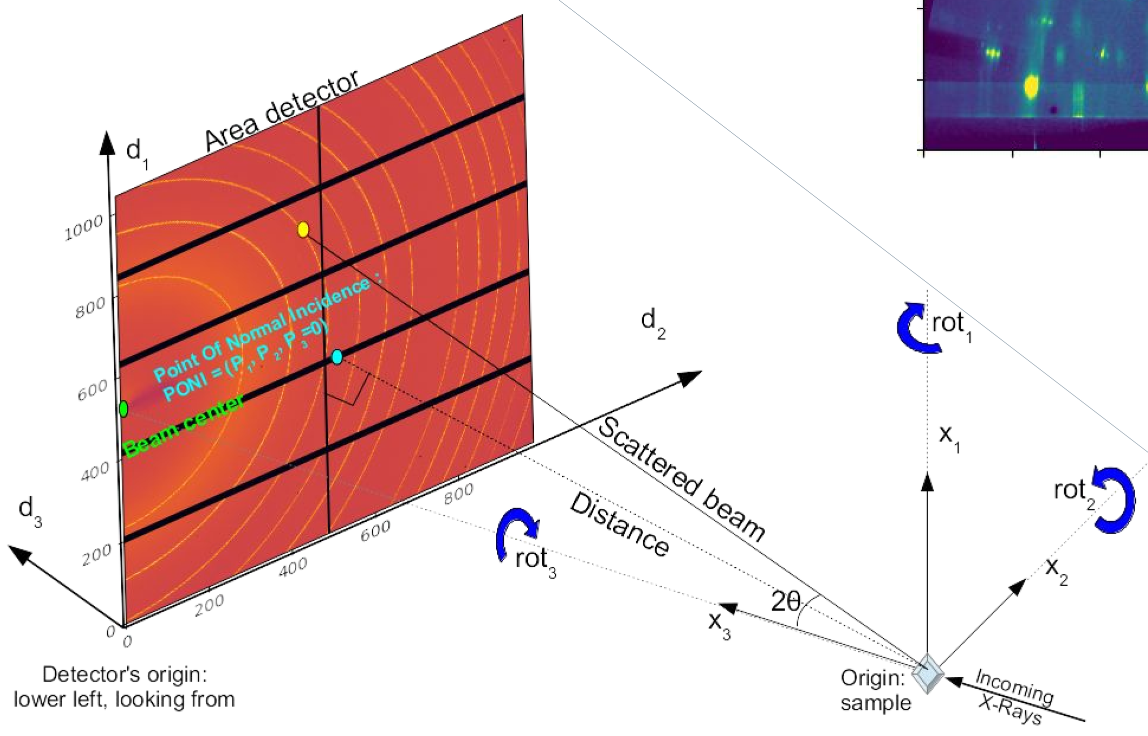
$$\vec{q}=\vec{q}_x(beam)+\vec{q}_y(horz)+\vec{q}_z(vert)$$

$$q_{IP}=\sqrt{q_x^2+q_y^2} \qquad q_{OOP}=q_z$$

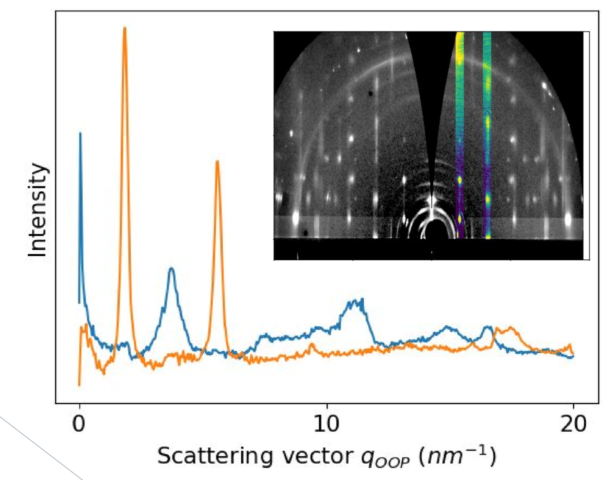



Missing wedge: the probed region of the reciprocal space is a sphere.

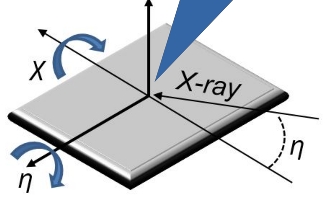
## Default orientation

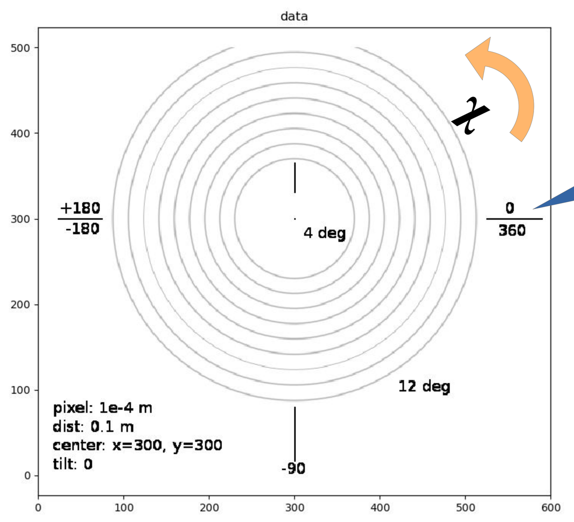



· ***1D-Integration along*** $\vec{q}$ ***components***



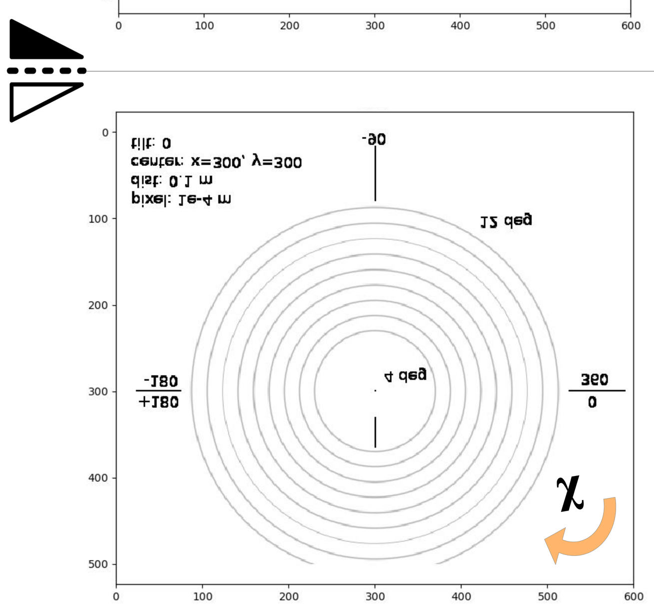

+ Incident angle (η)
+ Tilt angle (χ)



PyFAI has two convention for azimuthal range:
-180°→ +180°
0°→ +360°

Flip up/down



Native orientation of pyFAI:
- Look at the detector from the sample
- Origin is at the bottom of of the image
- The azimuth value turns in the trigonometric way

Native orientation of Dioptas:
- Look at the detector from the sample
- Origin is at the top of of the image
- The azimuth value turns clockwise

PONI-files have now an "orientation" tag for all detectors, which allows to handle the detector flipping:

1) Looking at the sample, origin a the top
2) Looking at the detector, origin at the top
3) Looking at the detector, origin at the bottom (default)
4) Looking at the sample, origin a the bottom

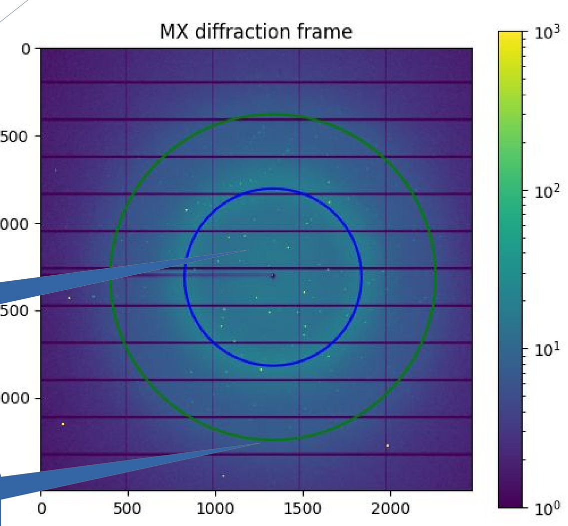
Radial units are properly converted.
Azimuthal angle cannot be converted !

Brings compatibility with Dioptas

**Limitations:**
Not yet for spline-file nor HDF5 defined detectors

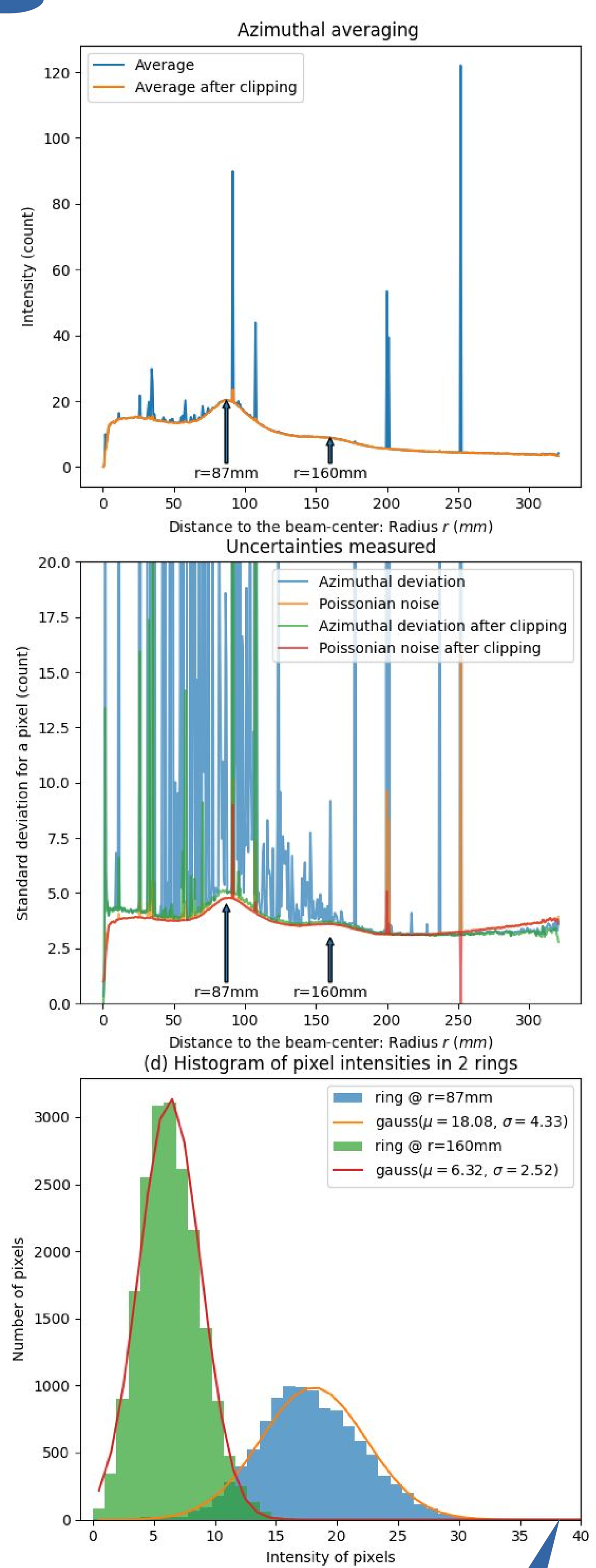
**PyFAI v2024.09**

## Error model Sigma-clipping



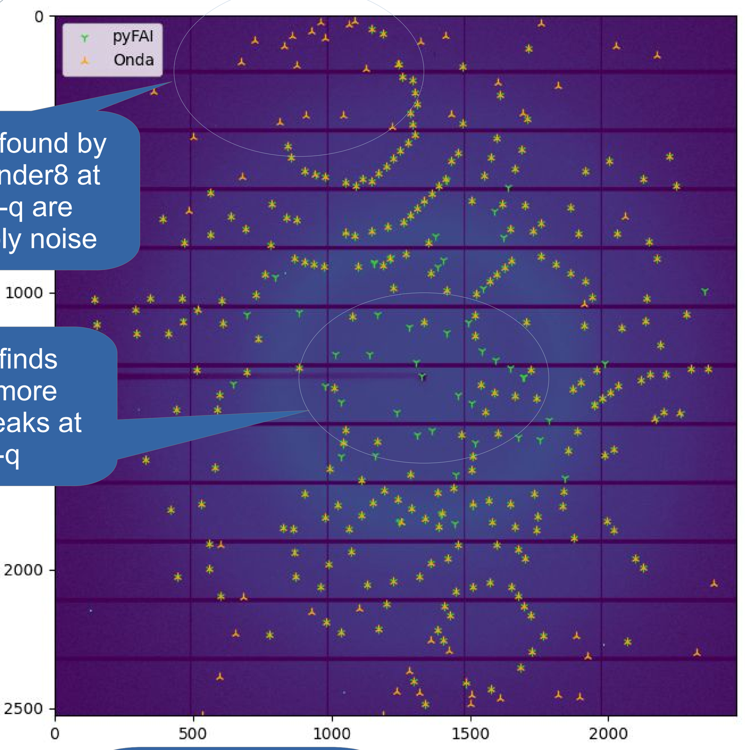

Bragg peaks on top of amorphous background

Rings at 87 & 160mm




Pixels at high-q are part of Bragg-peaks

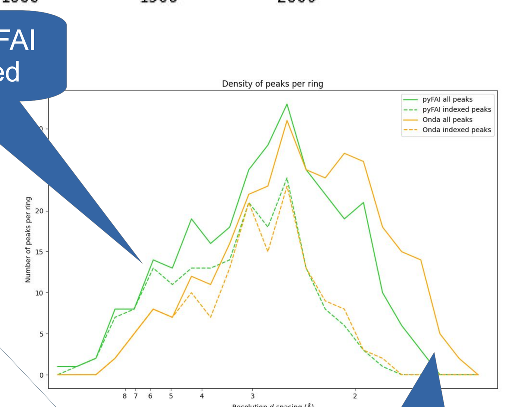
## Peak finding




Peaks found by Peakfinder8 at high-q are probably noise

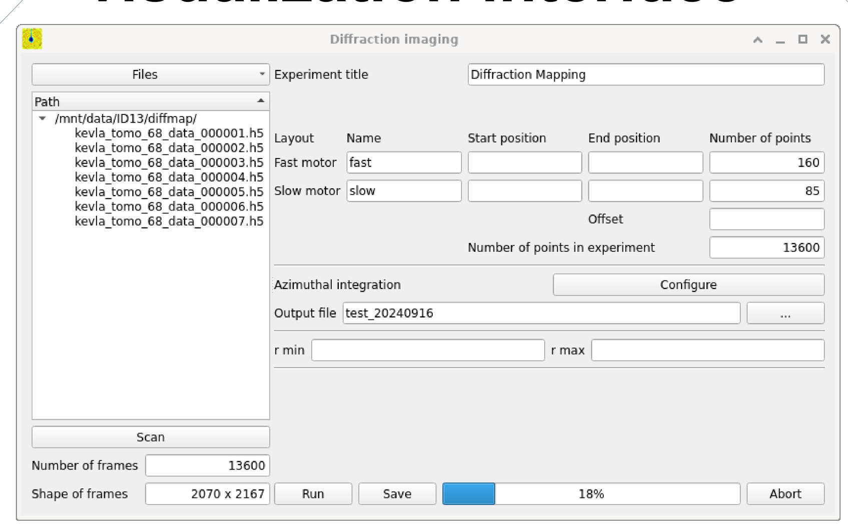
PyFAI finds many more Bragg peaks at low-q

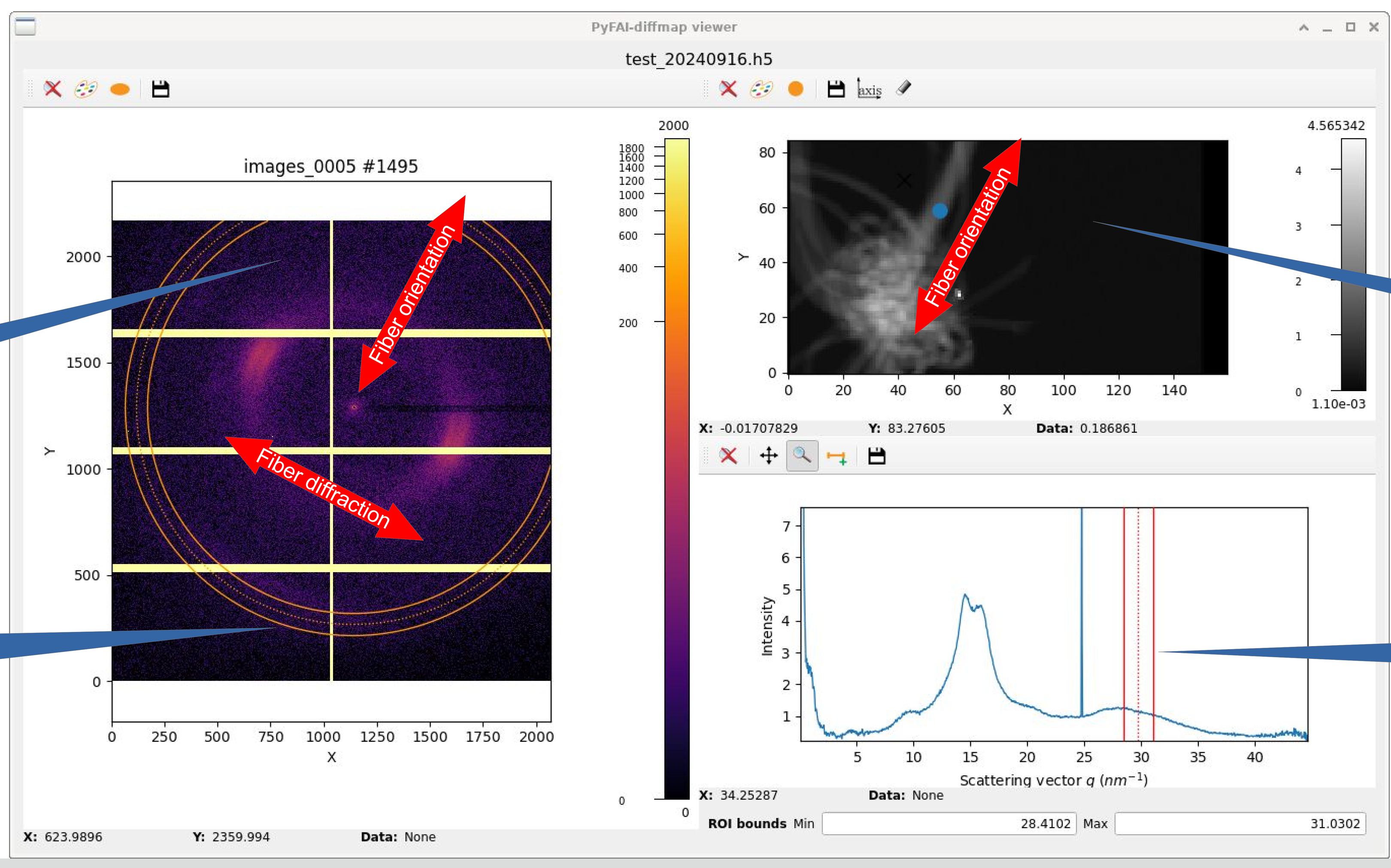
Peaks from pyFAI can be indexed



Peaks at high-q are indeed noise

## Diffraction map visualization interface




Diffraction image

Azimuthal Region Of Interest highlighted

Real space image obtained from a diffraction mapping experiment

Integrated (1d) powder pattern with Region Of Interest selectable

Pilx Graphical user interface

Kevlar knot dataset acquired on ID13

## What's next ?

- Median filtering in azimuthal space with pixel splitting
- Geometry exchange with *dioptas, crystfel, xds, ...*
- Optimization of geometry in q-space rather than 2theta for faster calibration
- Reach the Holy Grail: NoBugs !

[1] J. Kieffer, V. Valls, N. Blanc and C. Hennig; Journal of Synchrotron Radiation (2020) 27 (2), 558-566
[2] J. Kieffer, J. Orlans, N. Coquelle, S. Debionne, S. Basu, A. Homs, G. Santoni and D. De Sanctis, Journal of applied Crystallography (2024), accepted

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