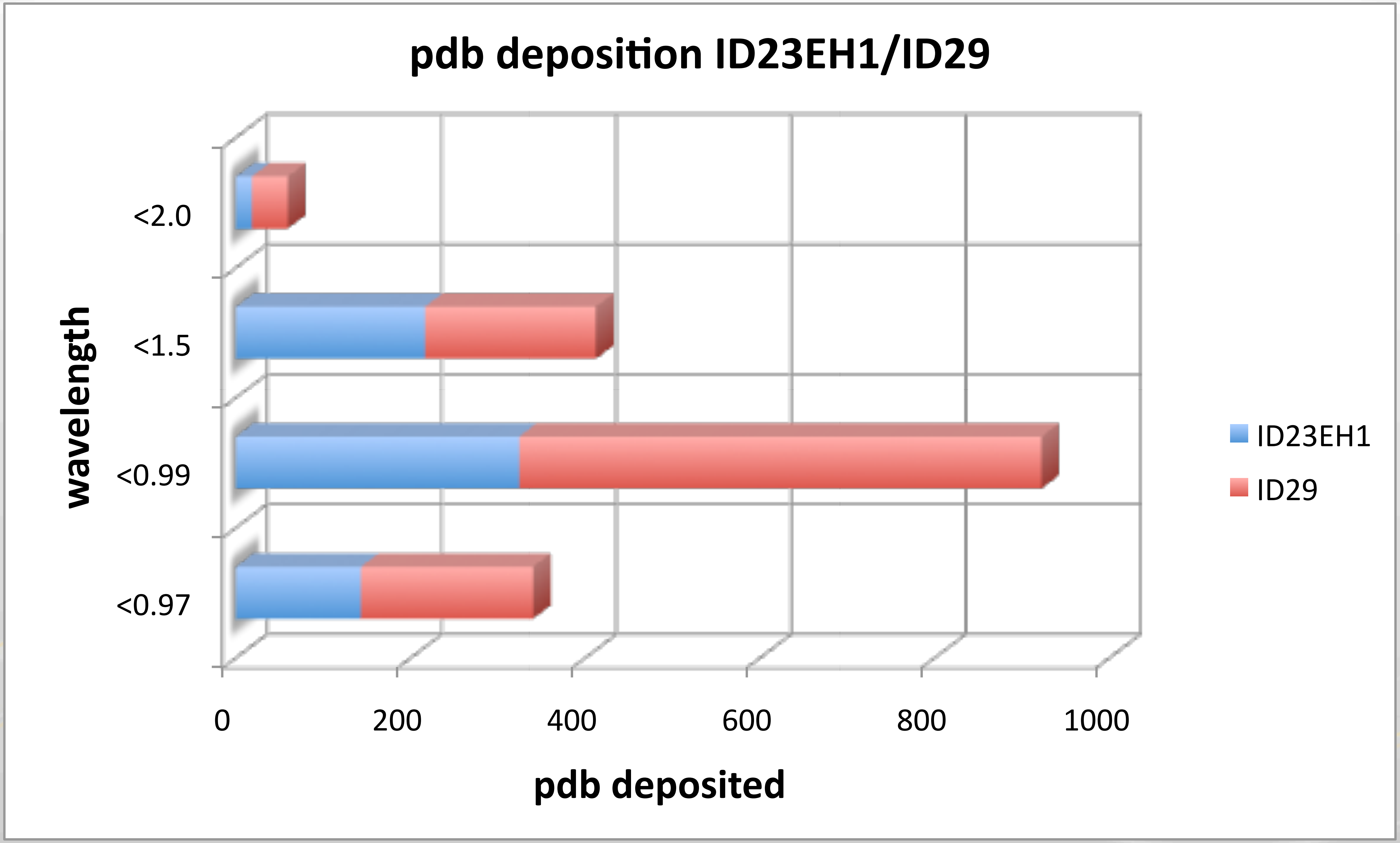
Longer wavelength setups at the ESRF

Outline

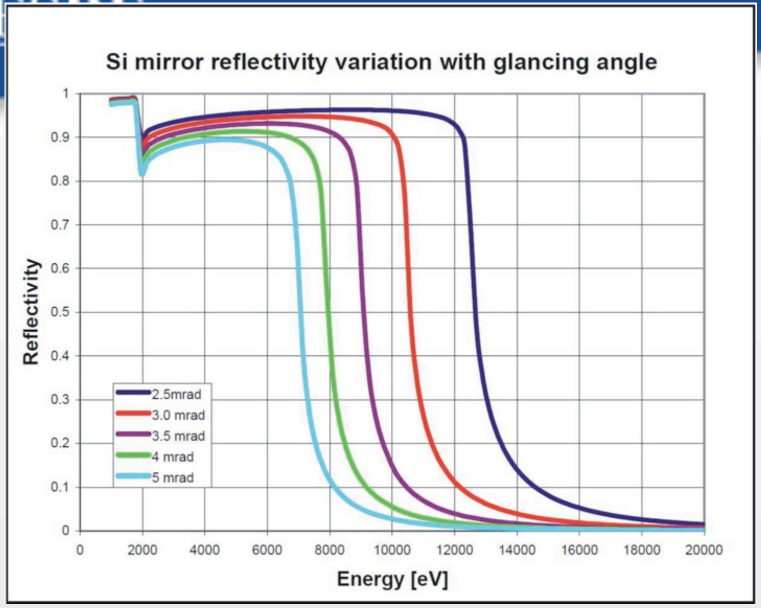
- Use of longer wavelength at ESRF
- ID29 overview
    - microbeam
    - Long Wavelength
- Current and future developments
    - Long Wavelength optimization
    - Integration with ID29S

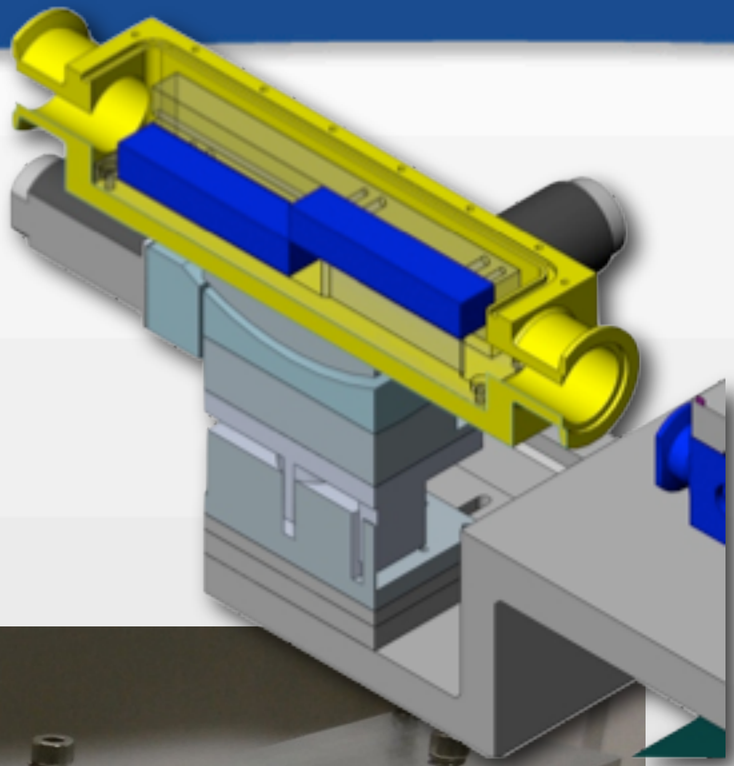

pdb deposition ID23EH1/ID29
wavelength
<2.0
<1.5
<0.99
<0.97
0
200
400
600
800
1000
pdb deposited
ID23EH1
ID29

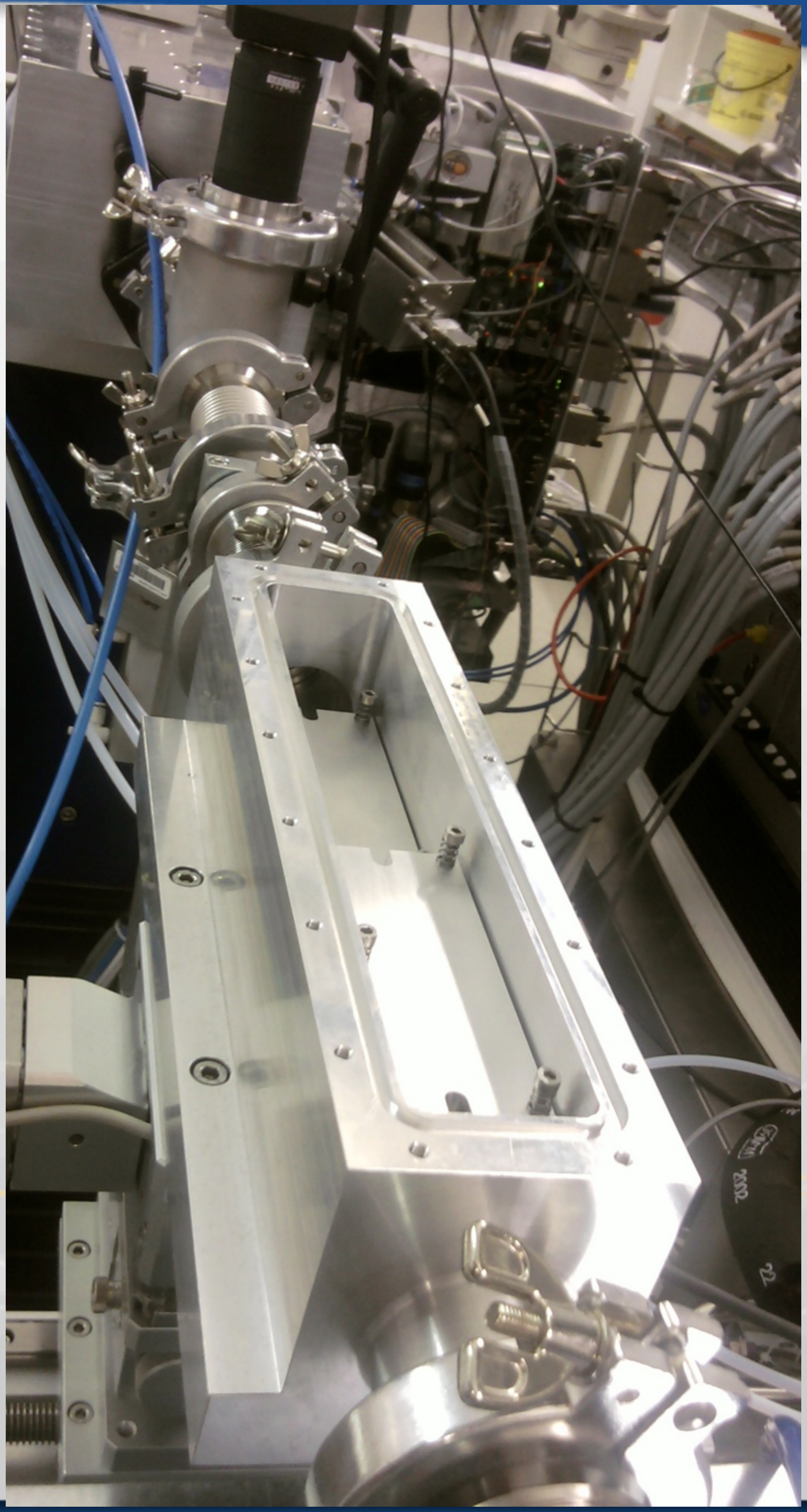
There are few *caveat* for a beamline to perform well at Long Wavelength

- 6 keV is contaminated by the 18 keV component
- Usually 3rd harmonic component is removed by detuning the second crystal, so less flux
- Photons delivery is severely limited by absorption of air, windows...

3rd harmonic removal



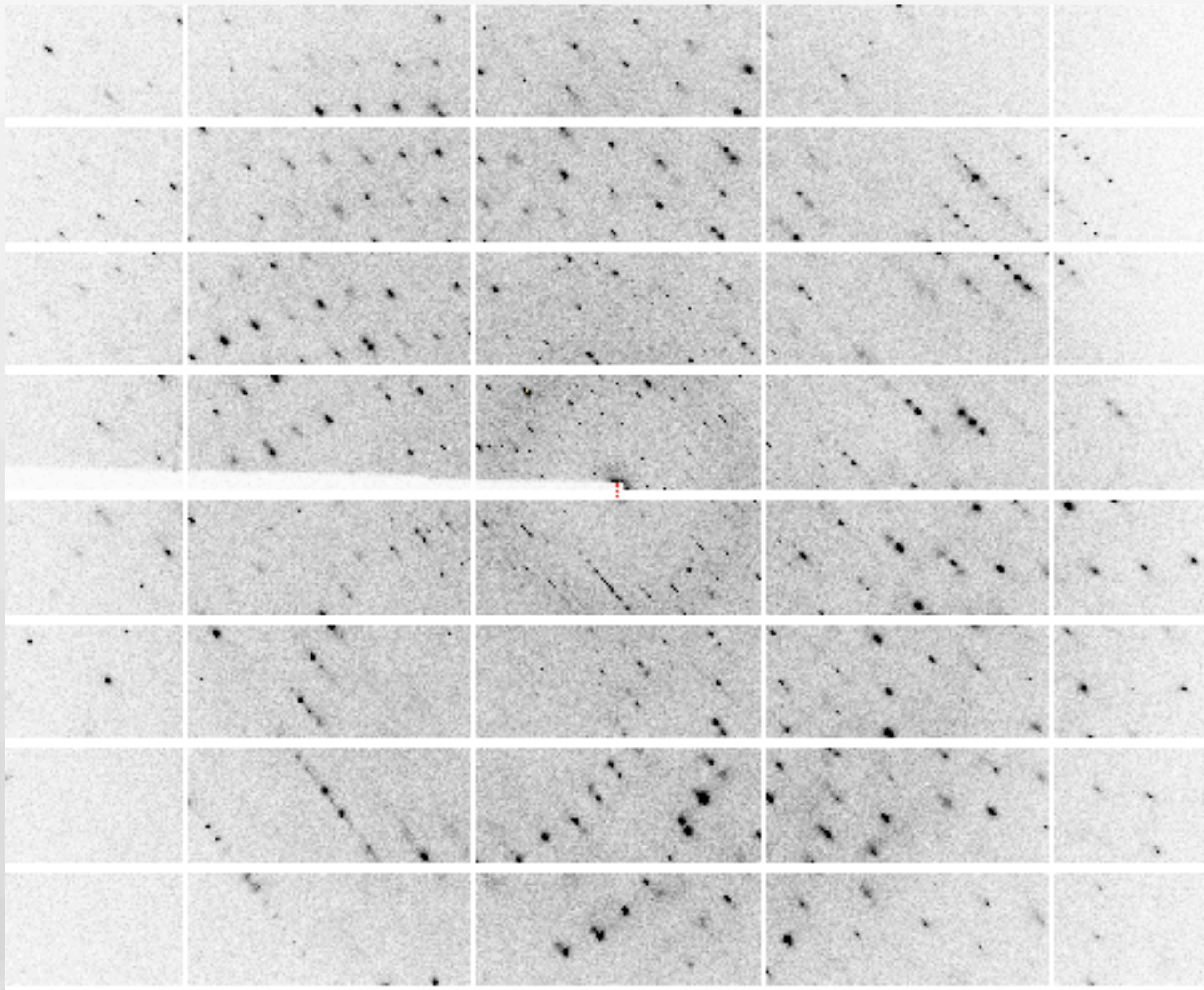




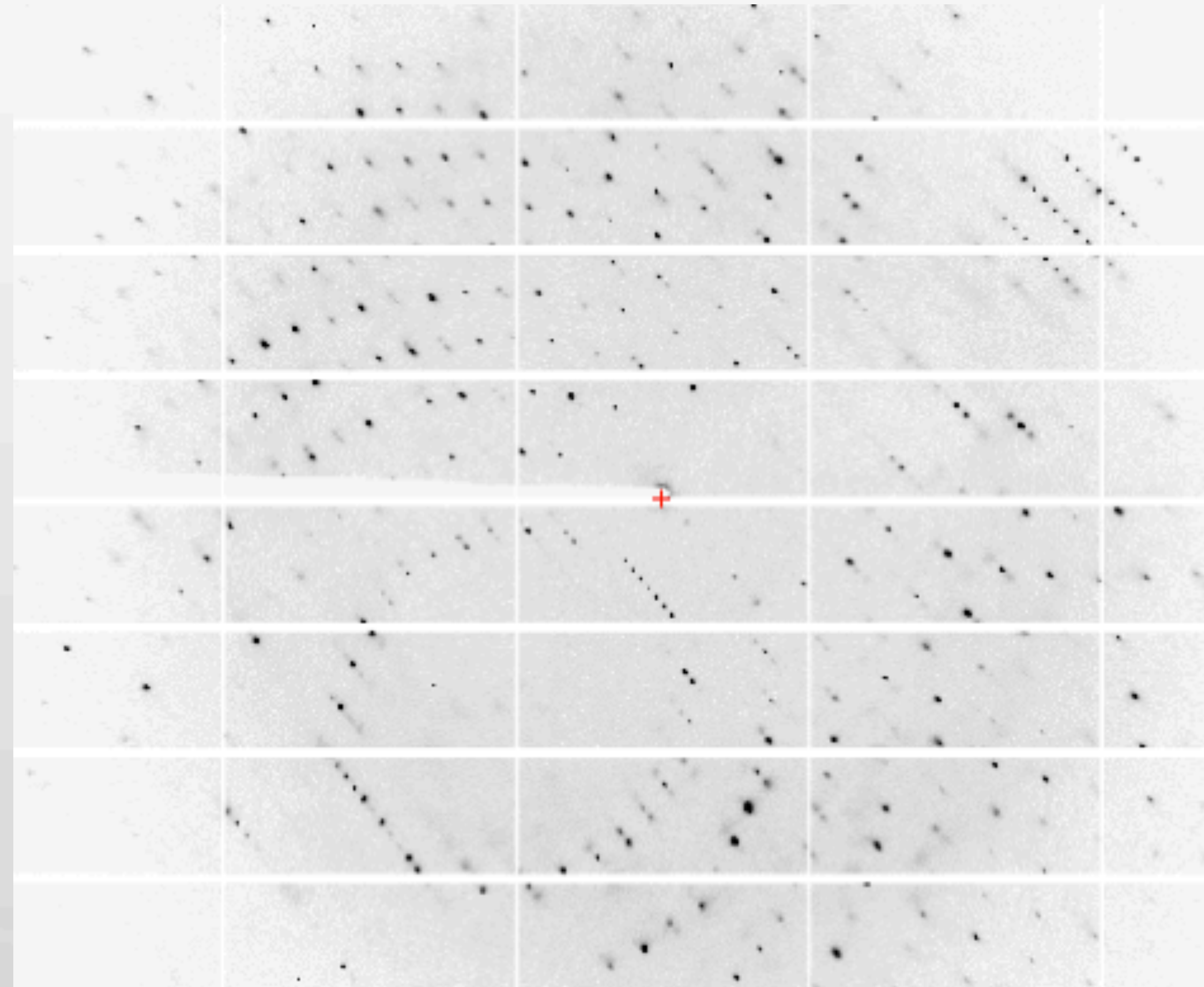
Two Si mirror to remove 3rd harmonic contamination

3rd harmonic removal

6 keV



6 keV with mirror

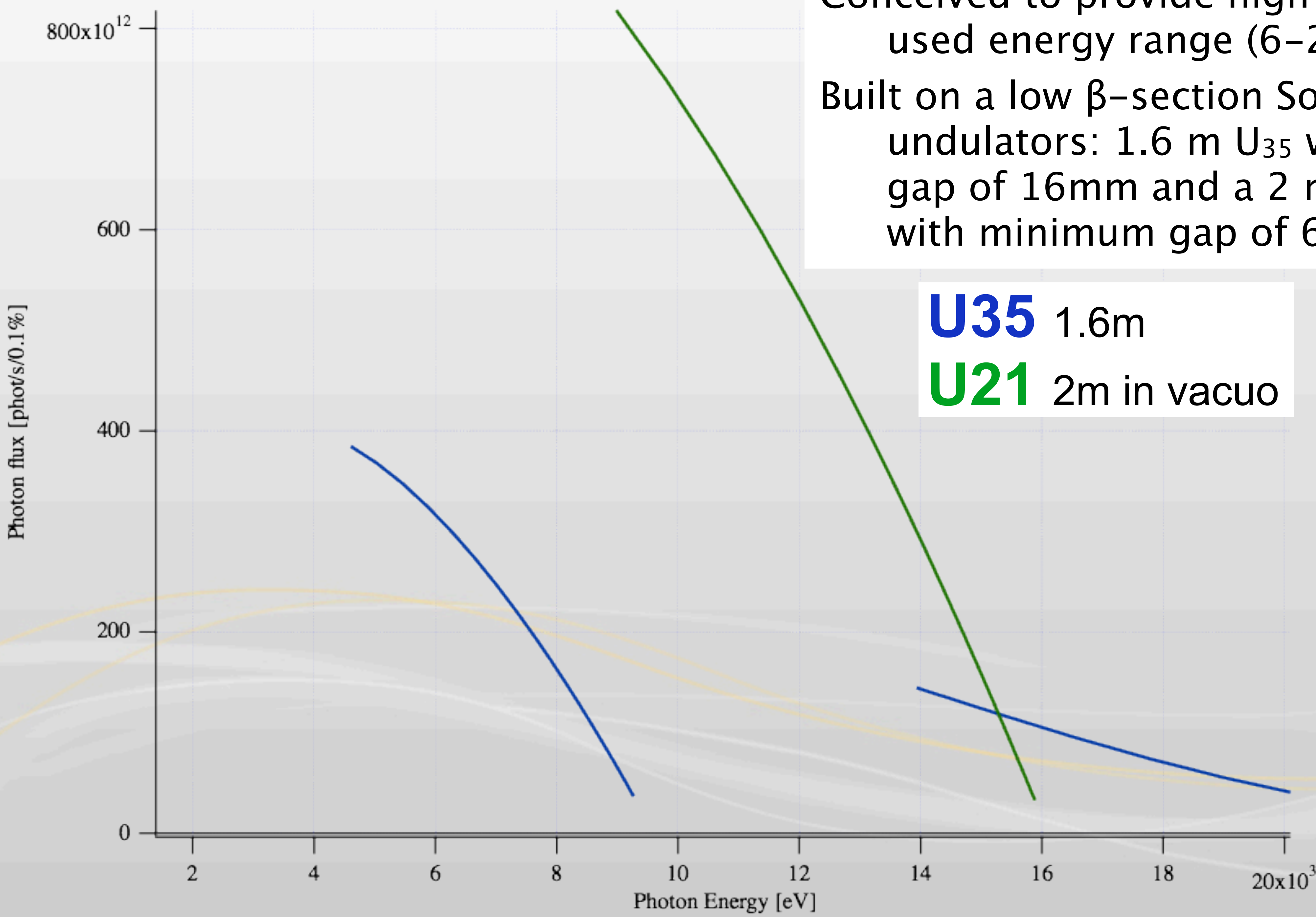


Decontamination from 3rd harmonic

Usually 3rd harmonic component is removed by detuning the second crystal - using of mirrors give 50% flux increase

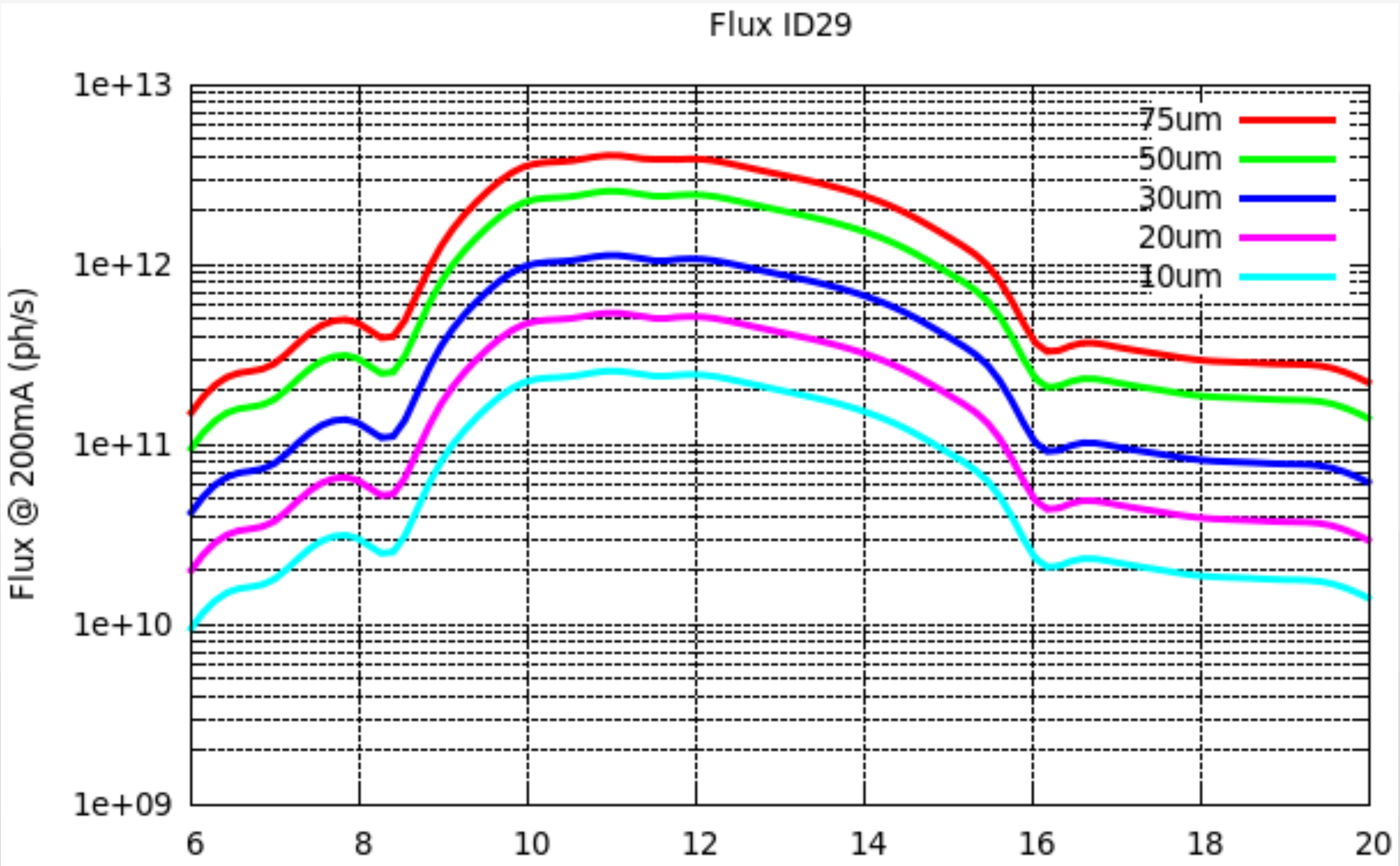
ID29 source

- Conceived to provide high flux over all used energy range (6-20 keV)
- Built on a low β-section Source are two undulators: 1.6 m U_{35} with minimum gap of 16mm and a 2 m in vacuum U_{21} with minimum gap of 6mm

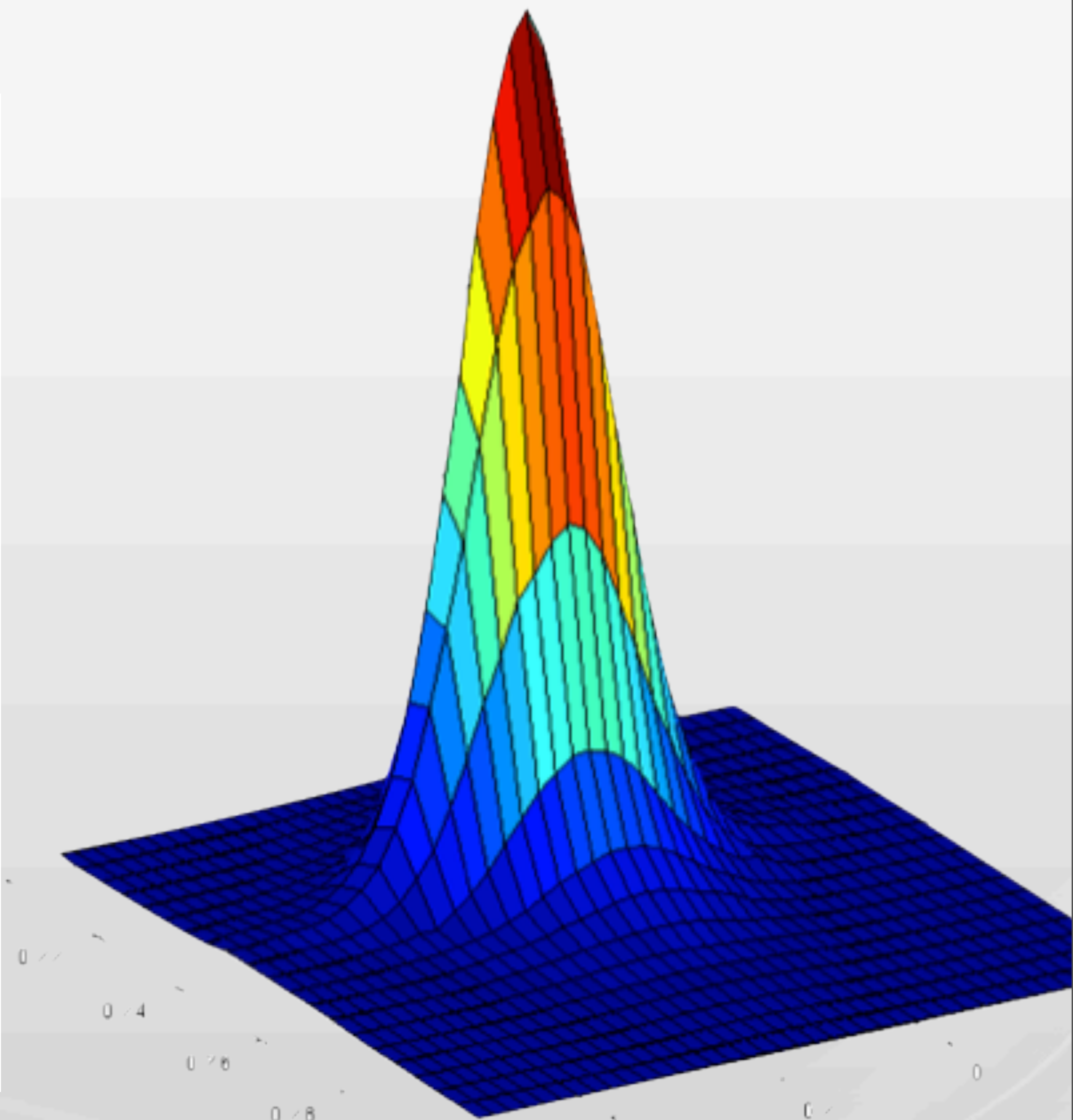


U35 1.6m
U21 2m in vacuo

Flux

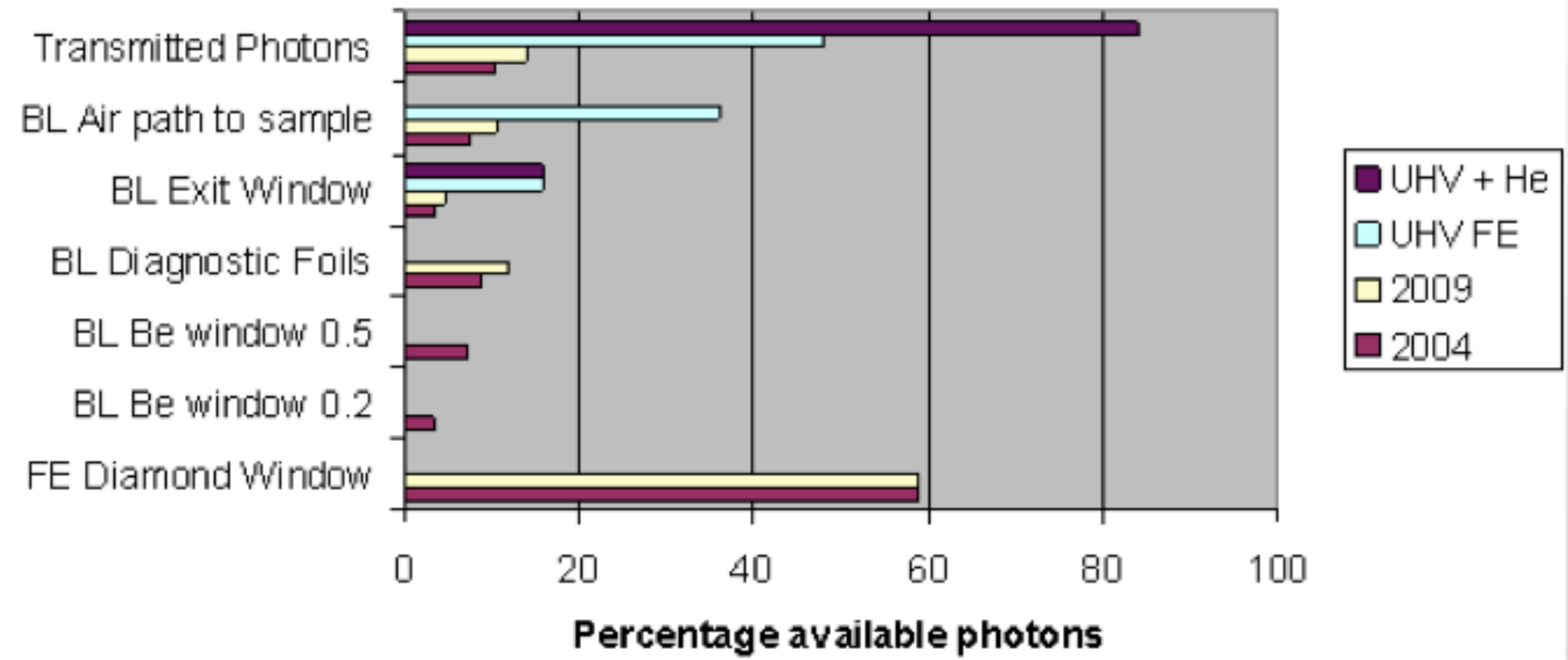


Flux at sample position vs Energy



More flux is needed, especially at long wavelength and on a small focus spot

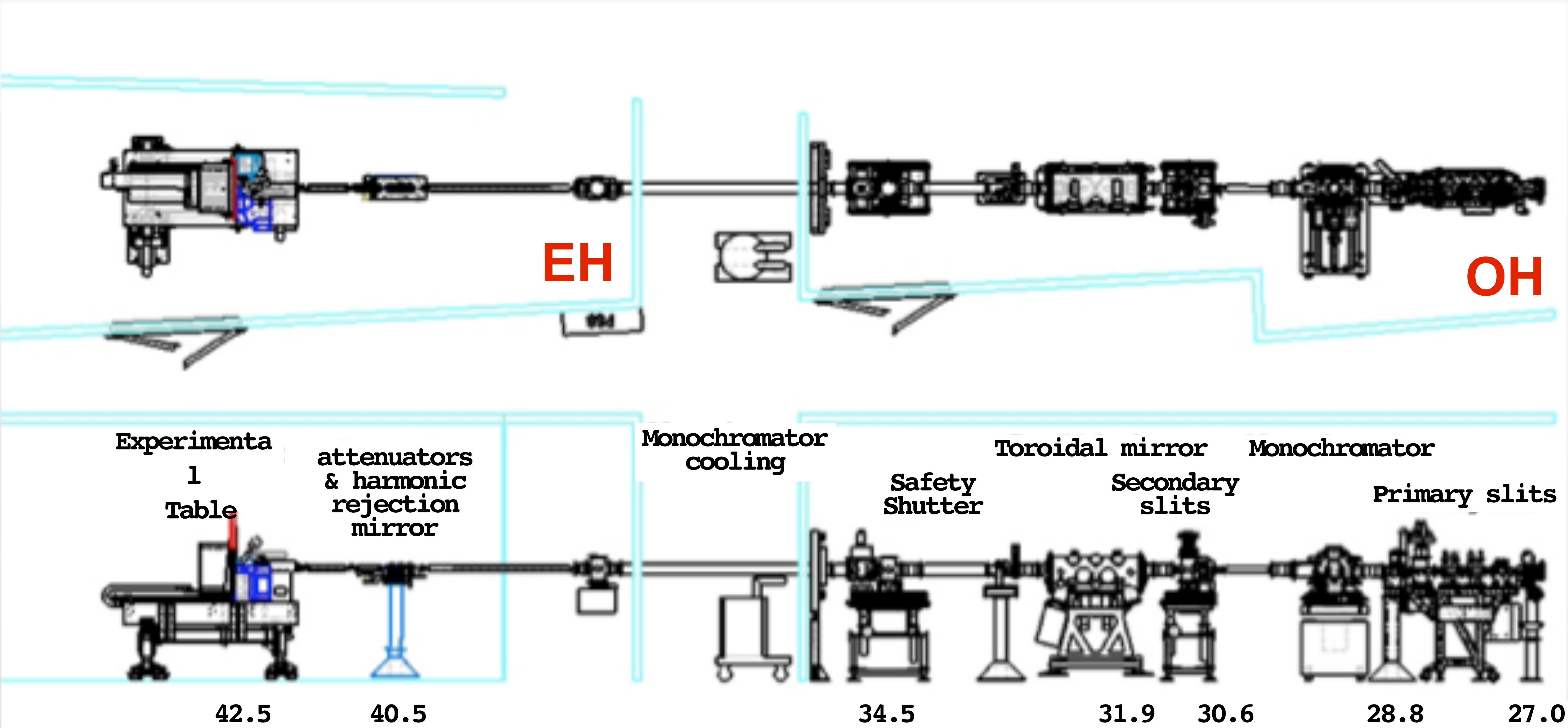
Absorption



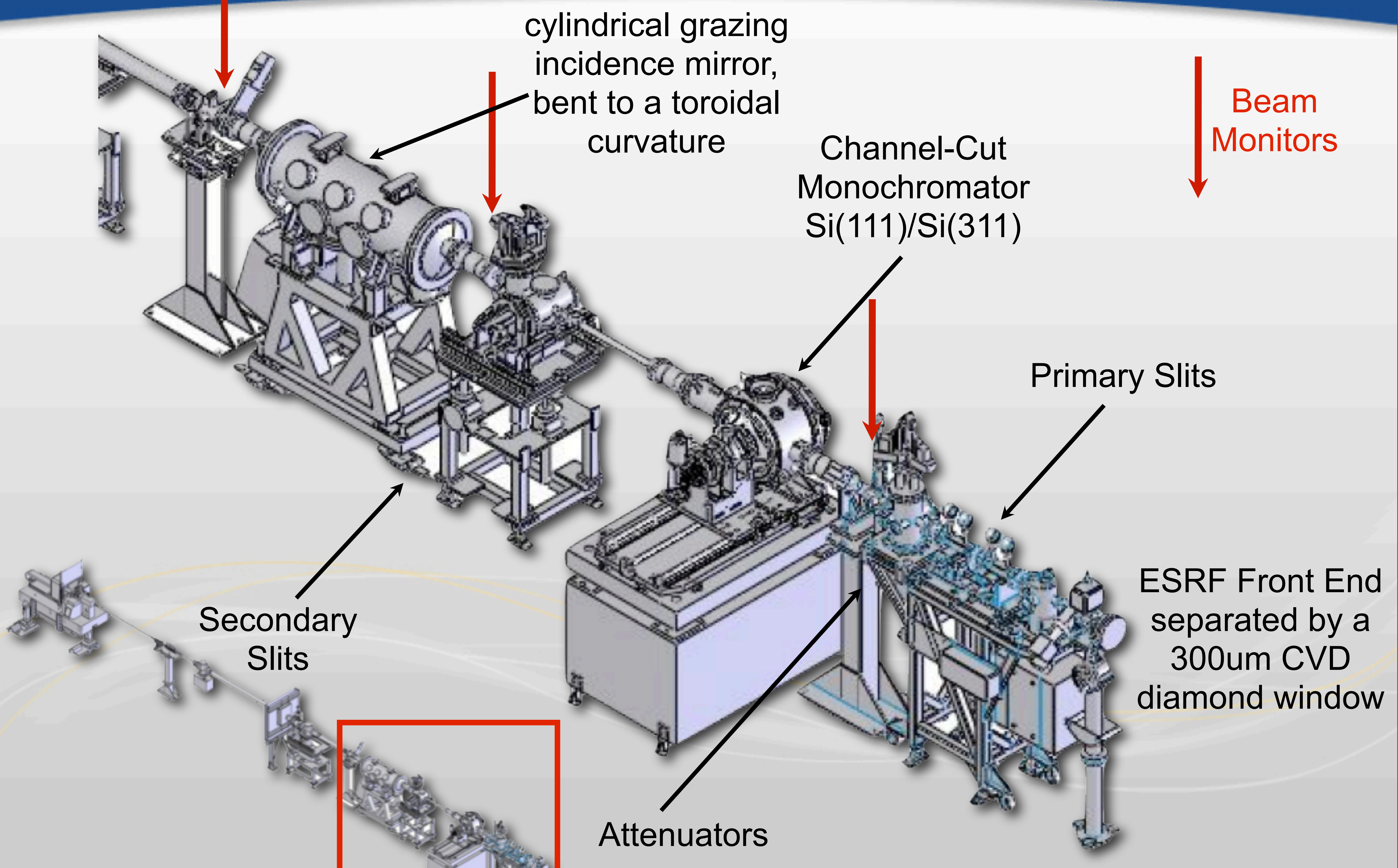
At current status only 15% of photons produced at 6keV arrive to the sample. Improvement are possible removing the CVD diamond of the FE and to reduce the beampath in air

ID29

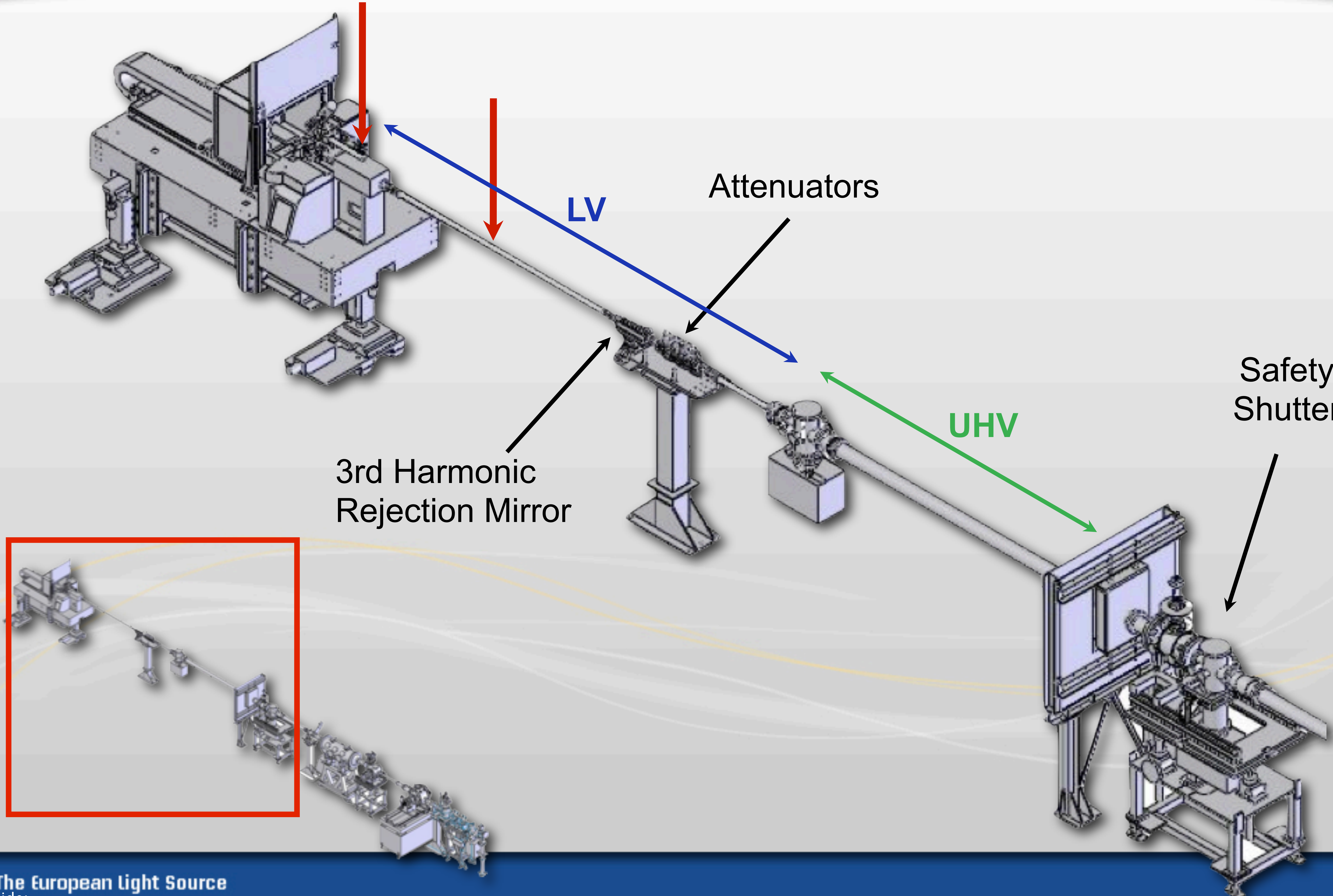
ID29 is divided in autonomous functioning sections to be simple to automate and align



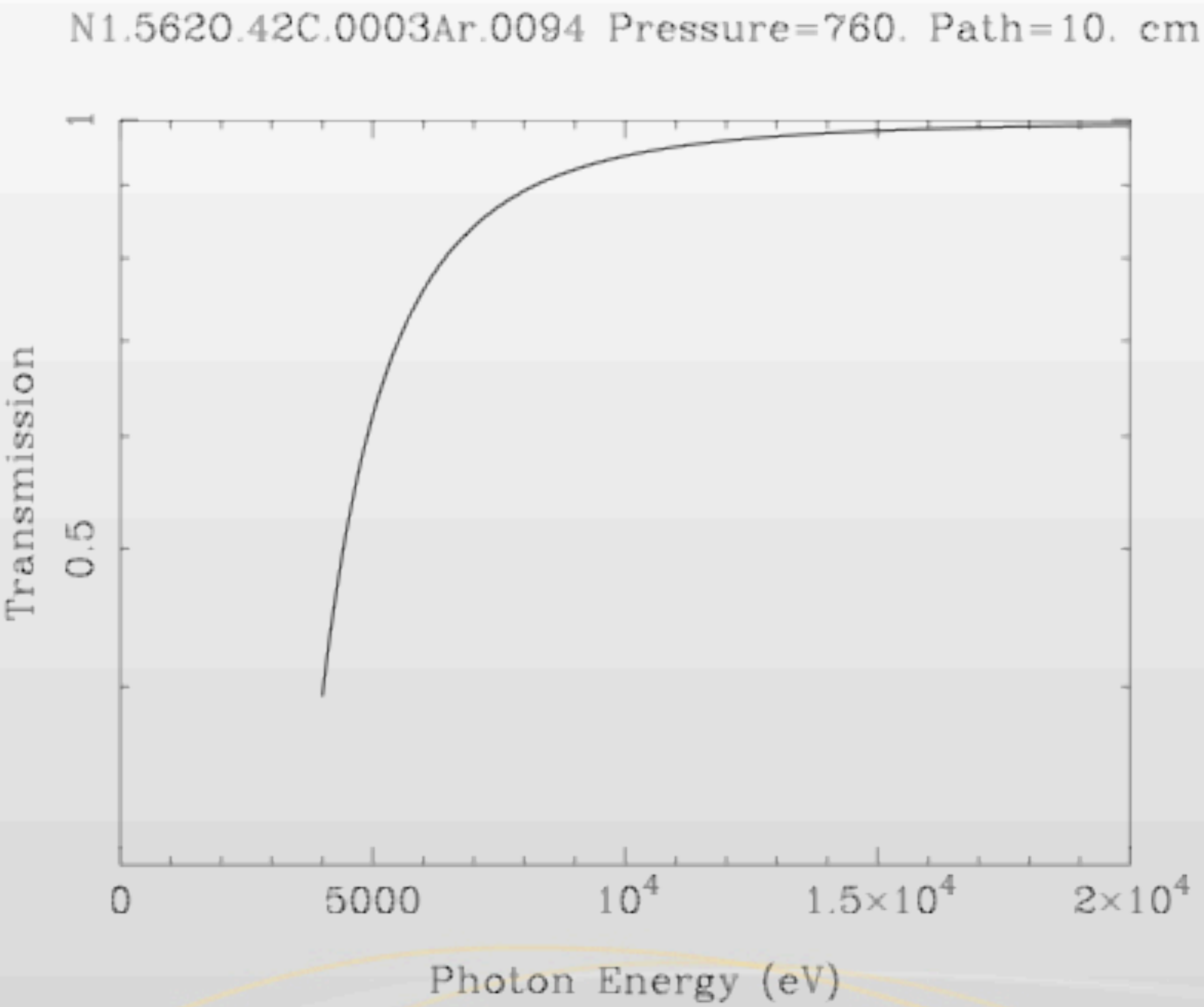
Optics Hutch

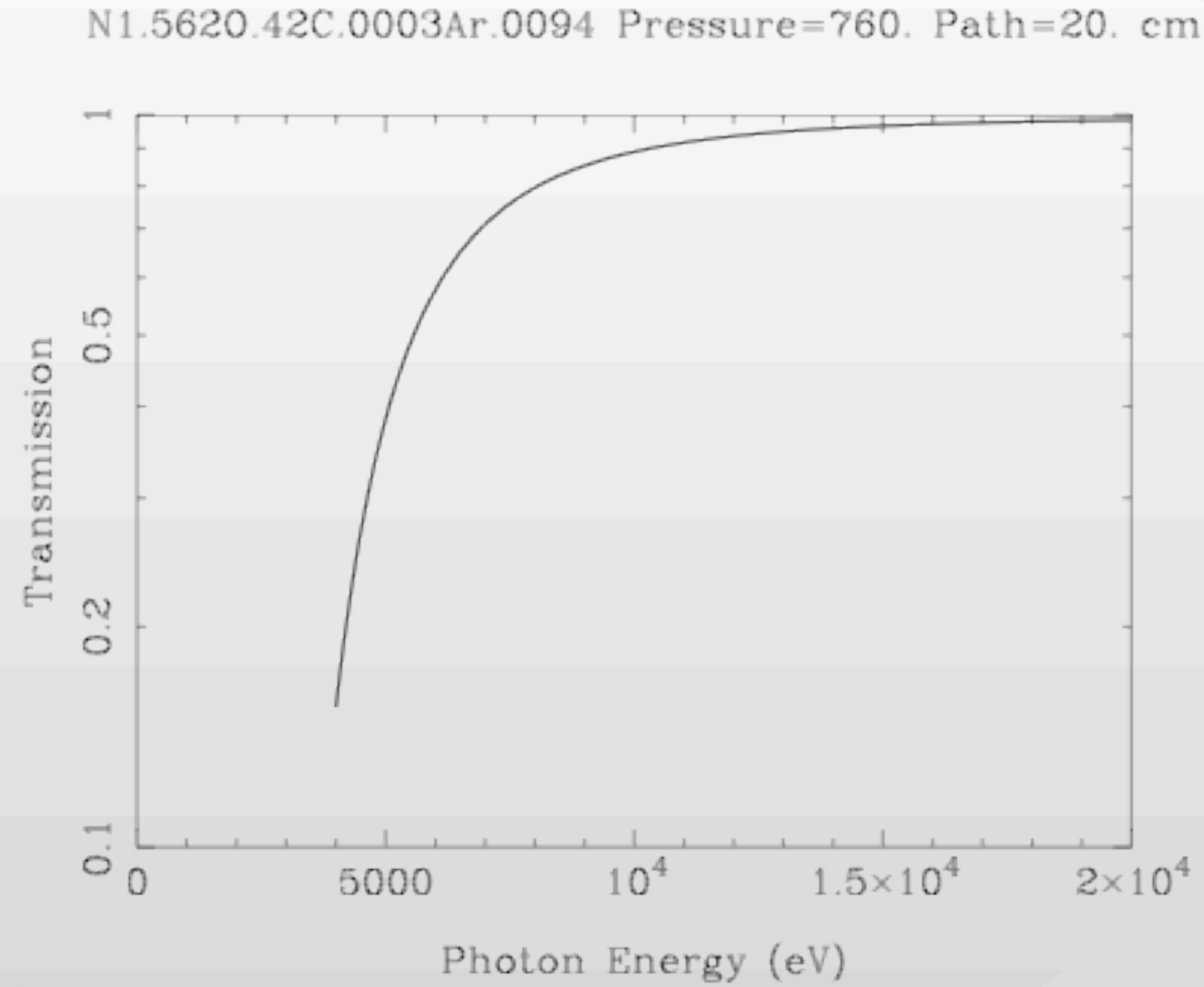


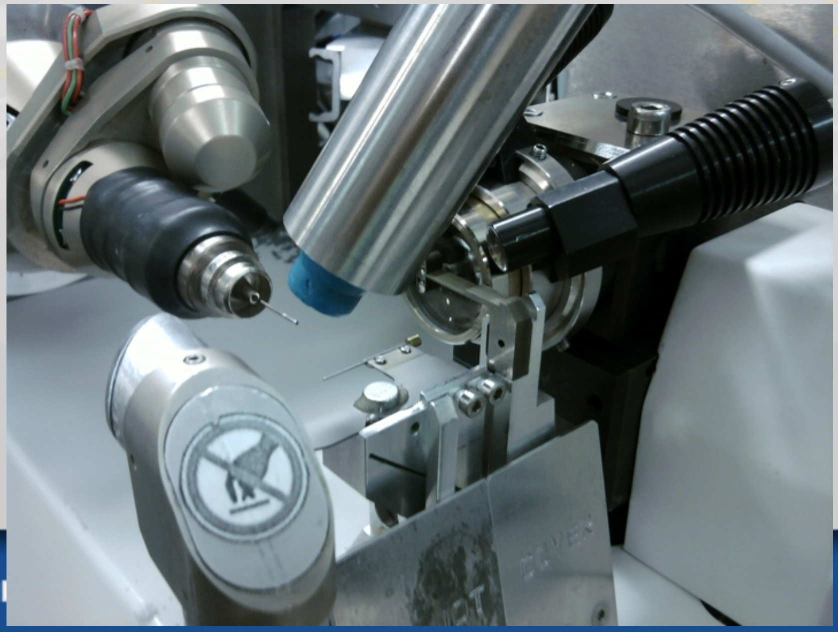
Experimental Hutch

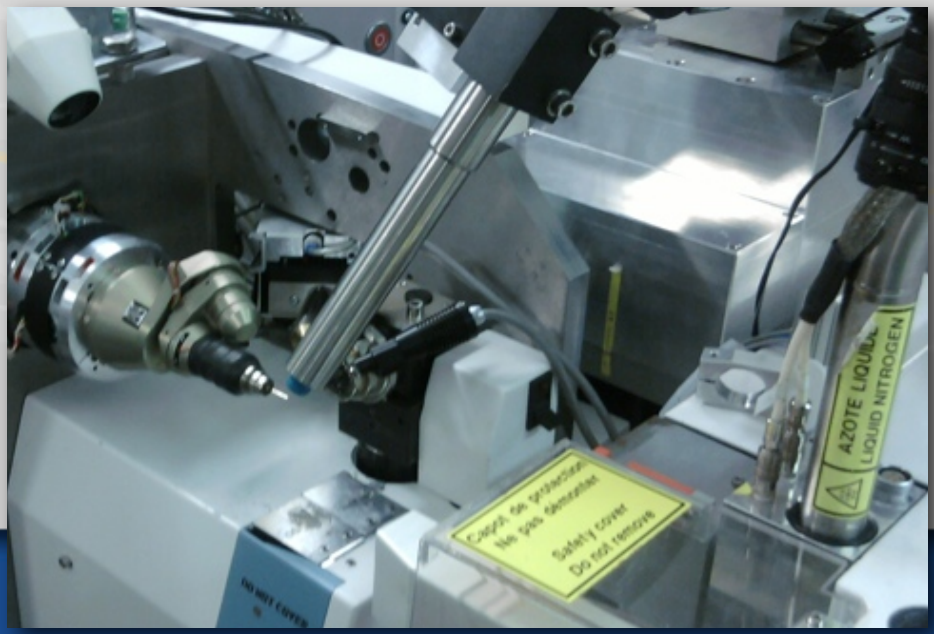


Air Absorption





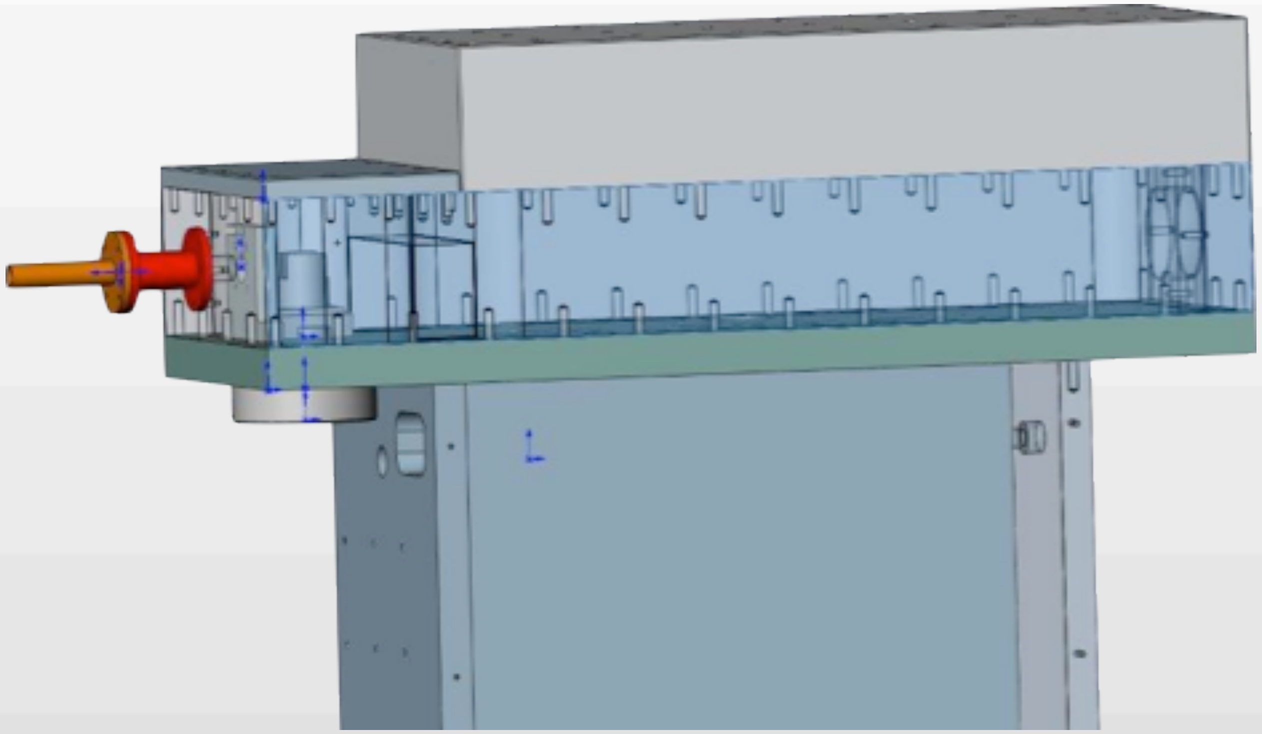


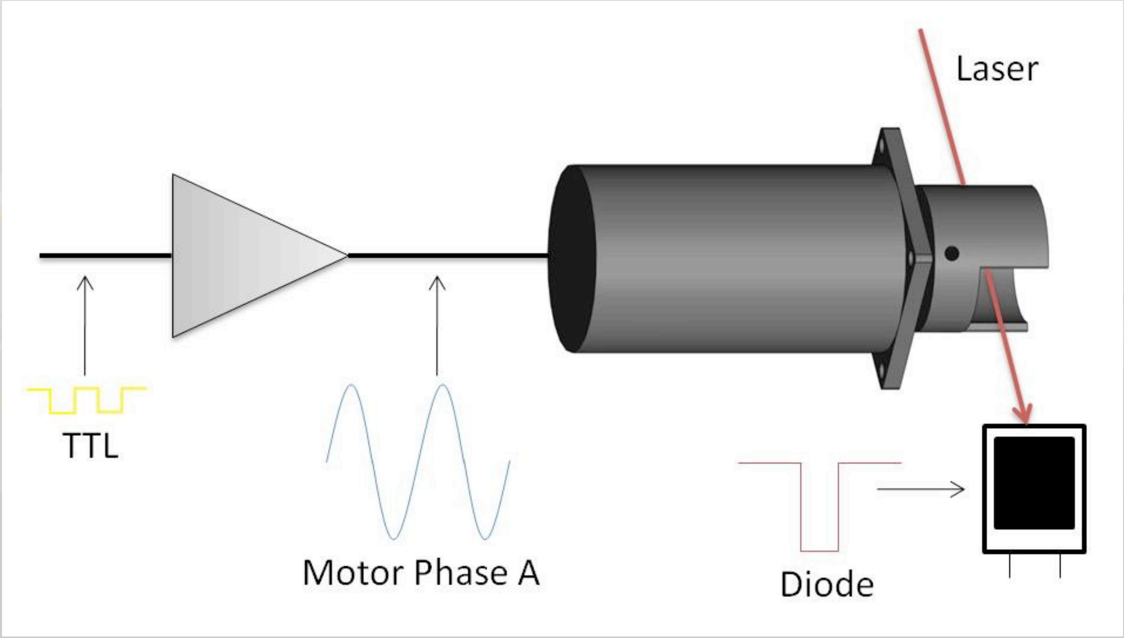


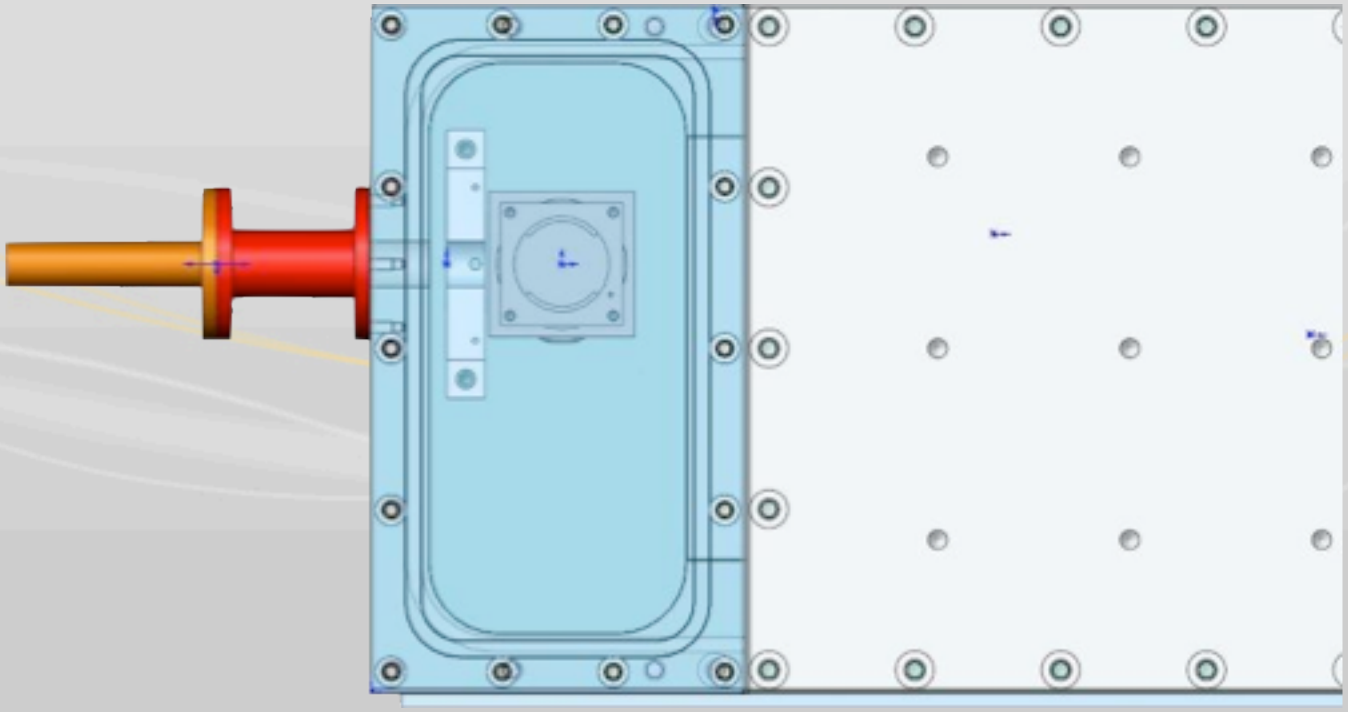
New slitbox+shutter

A new slitbox will extend the vacuum path to the back of the OAV

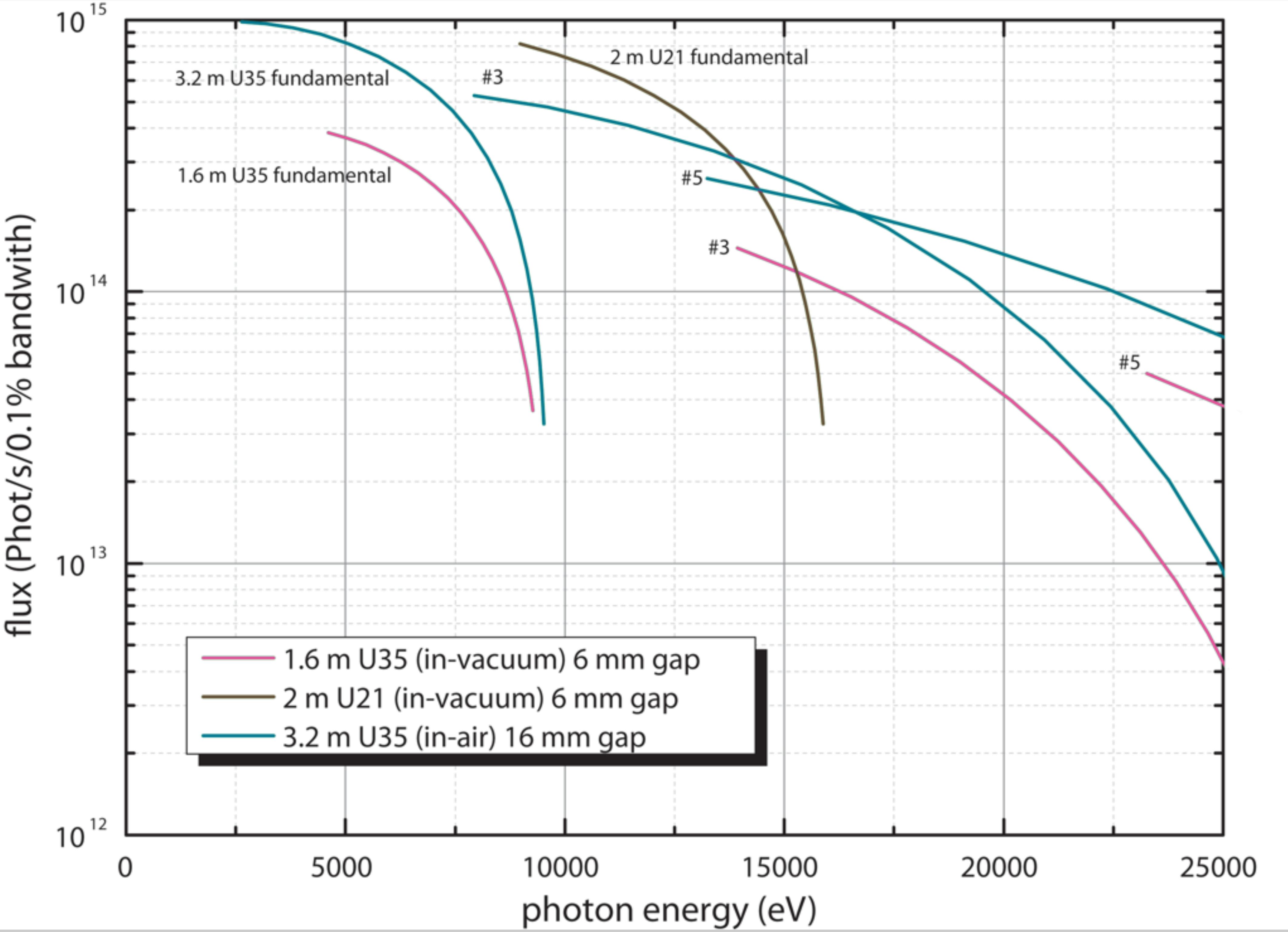
It will mount the new rotative shutter vacuum compatible



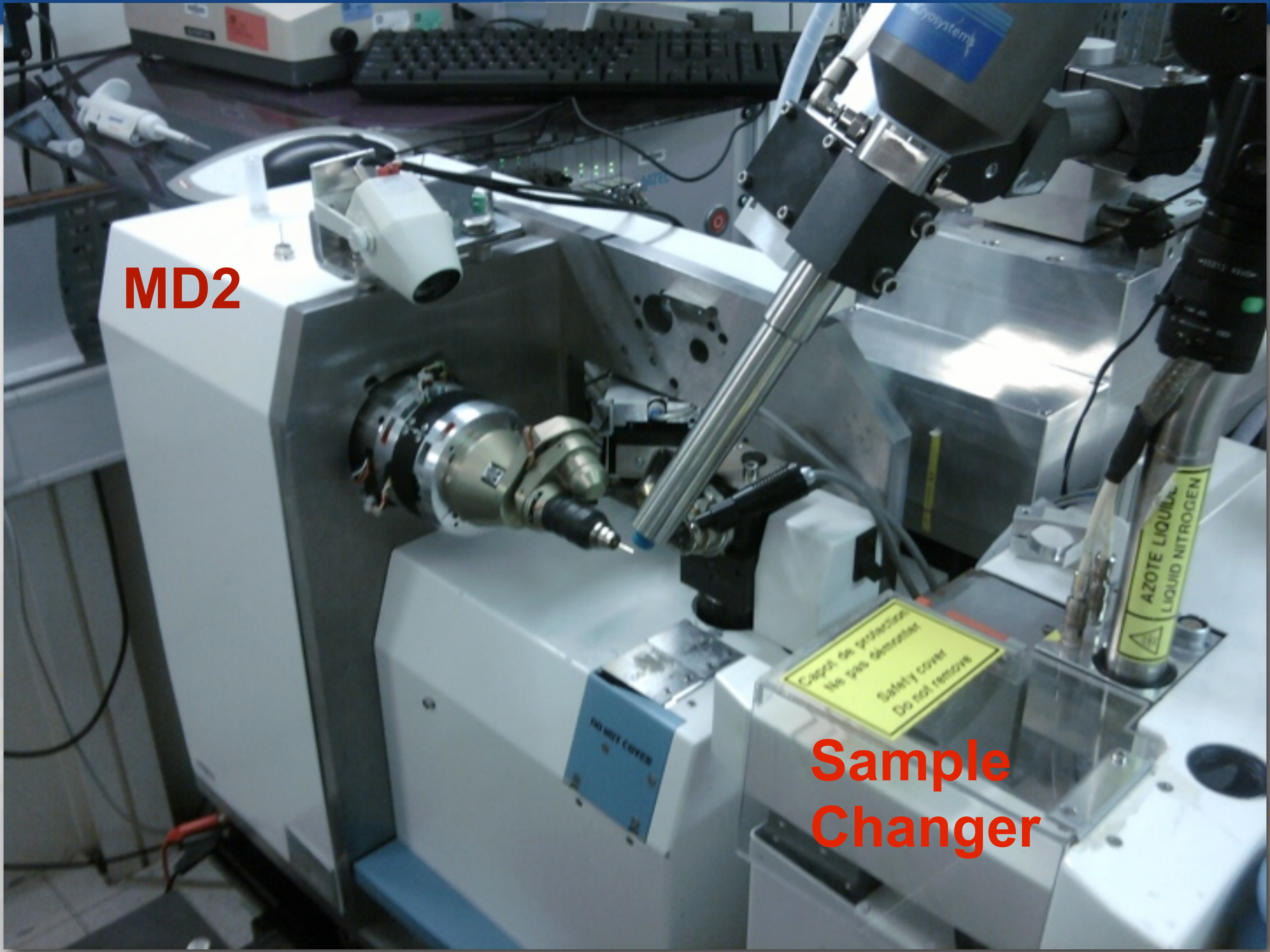




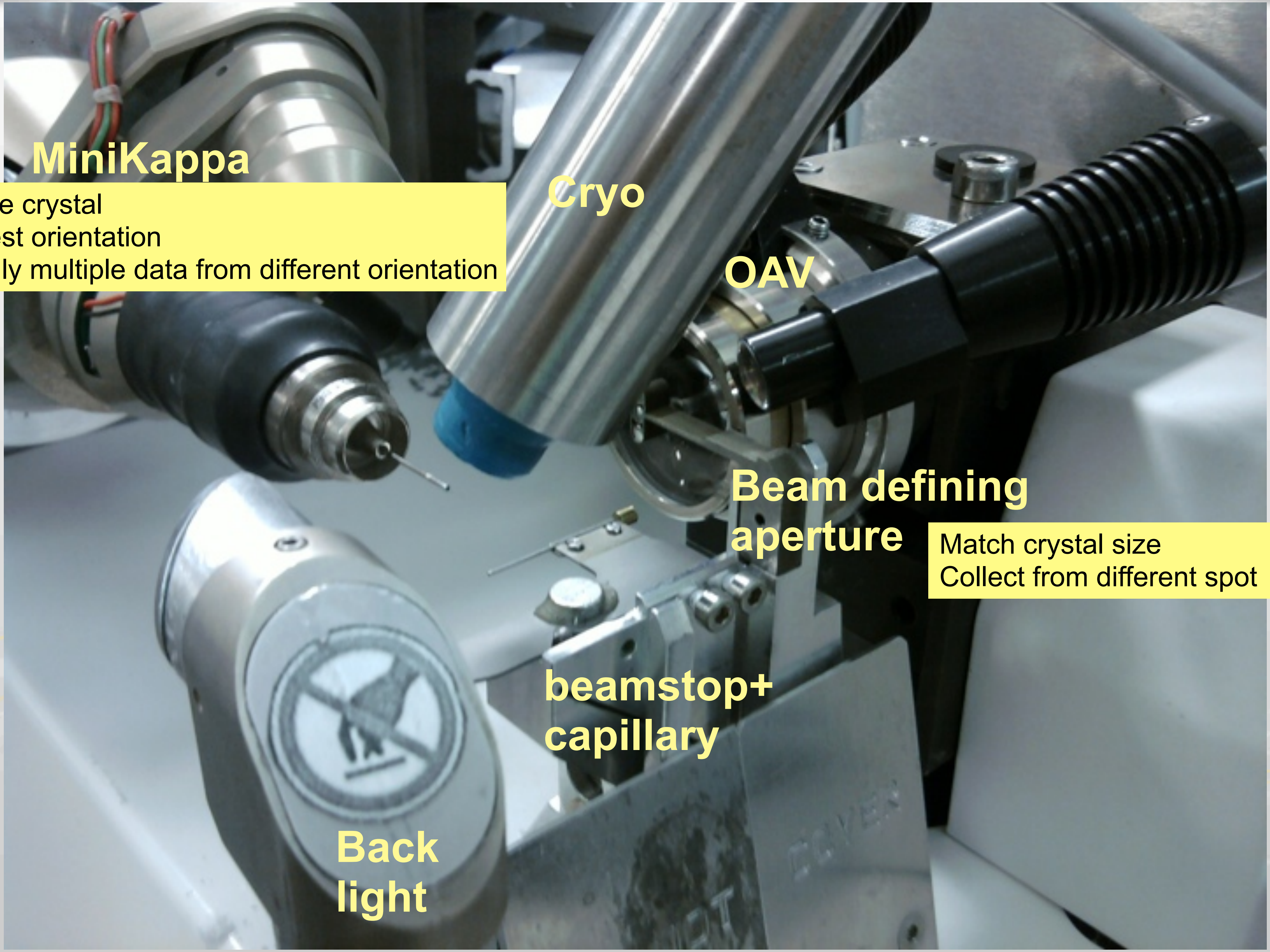
New undulator



Sample Environment



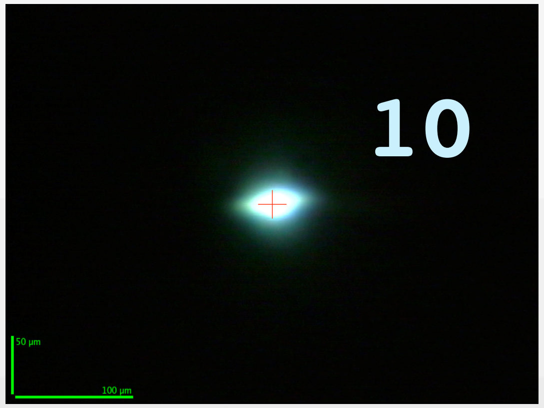
MD2

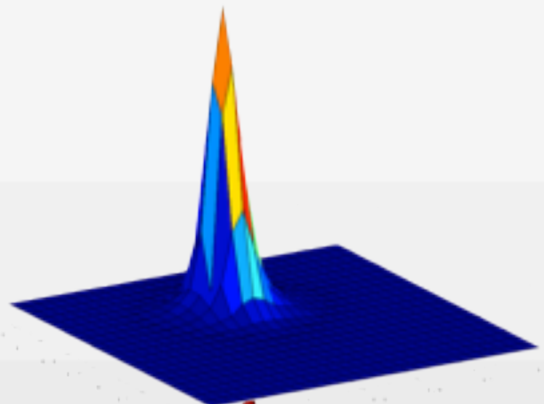


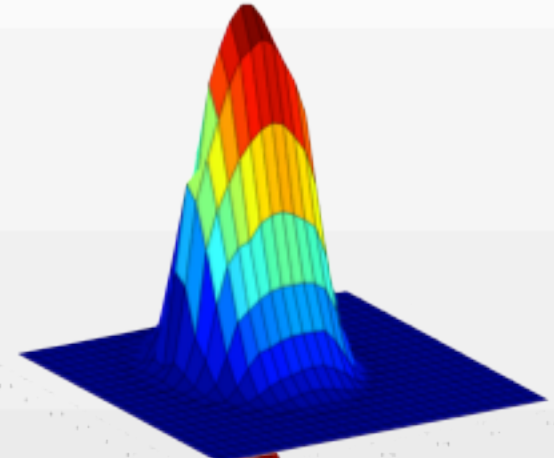
Reorient the crystal
Find the best orientation
Collect really multiple data from different orientation

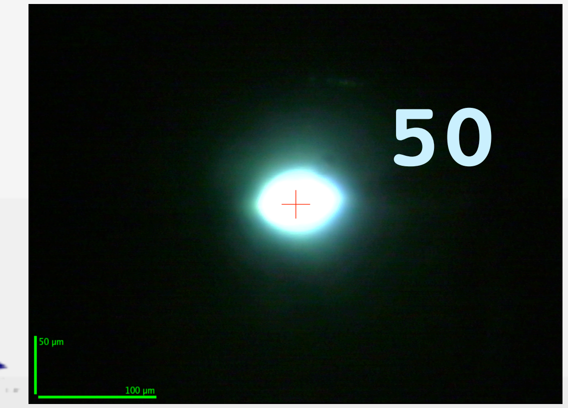
Match crystal size
Collect from different spot

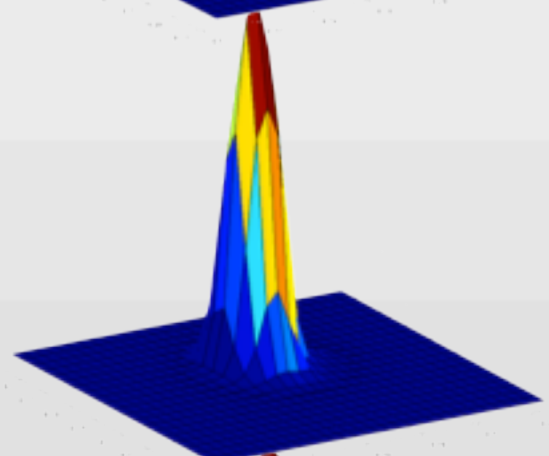
µbeam

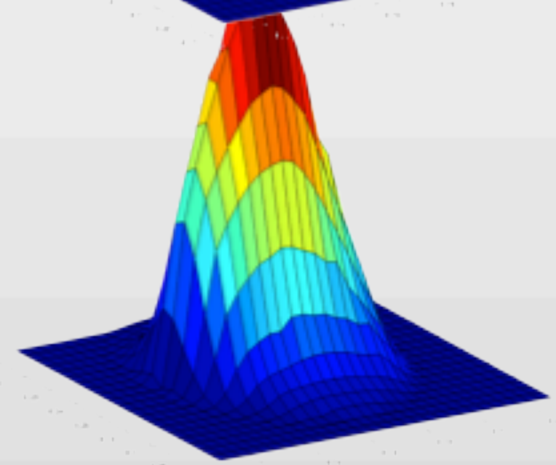


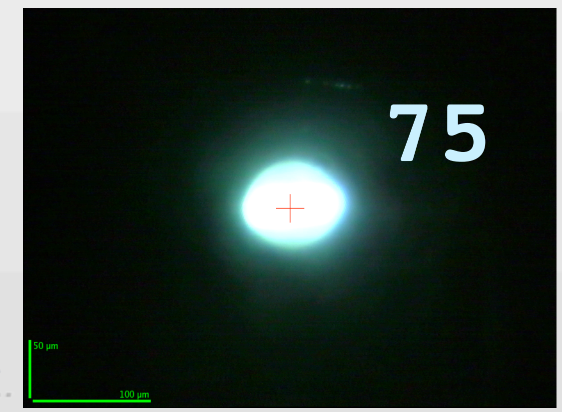


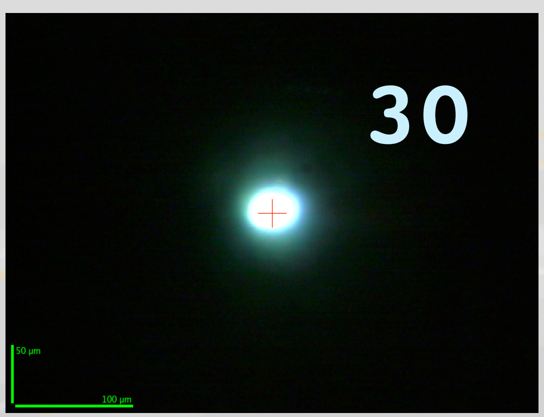


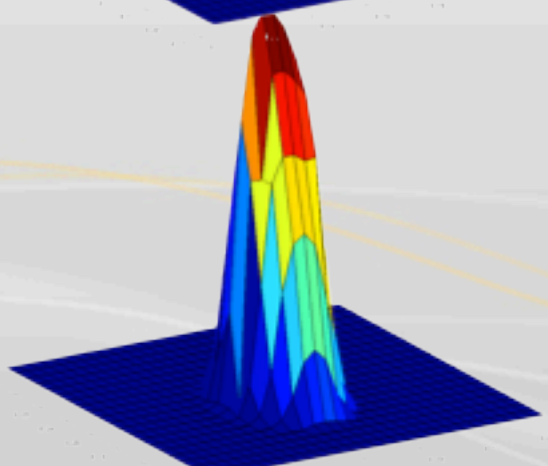


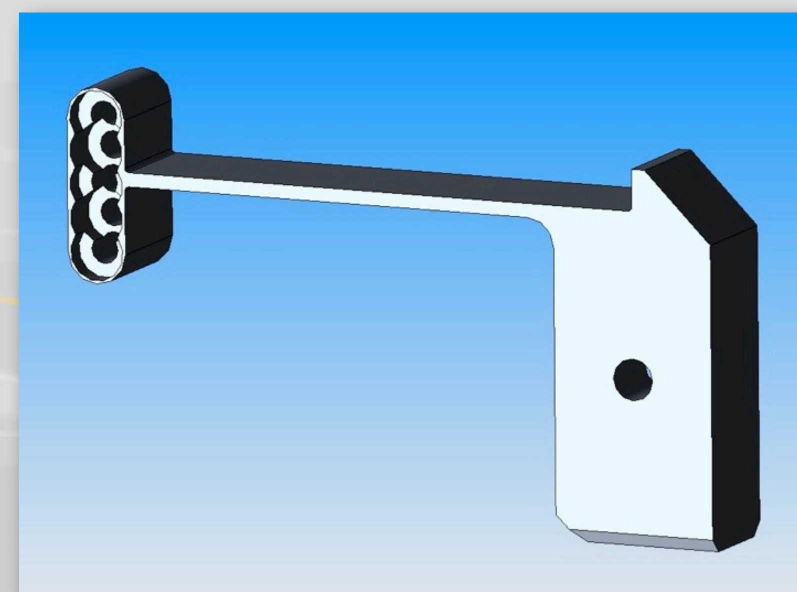






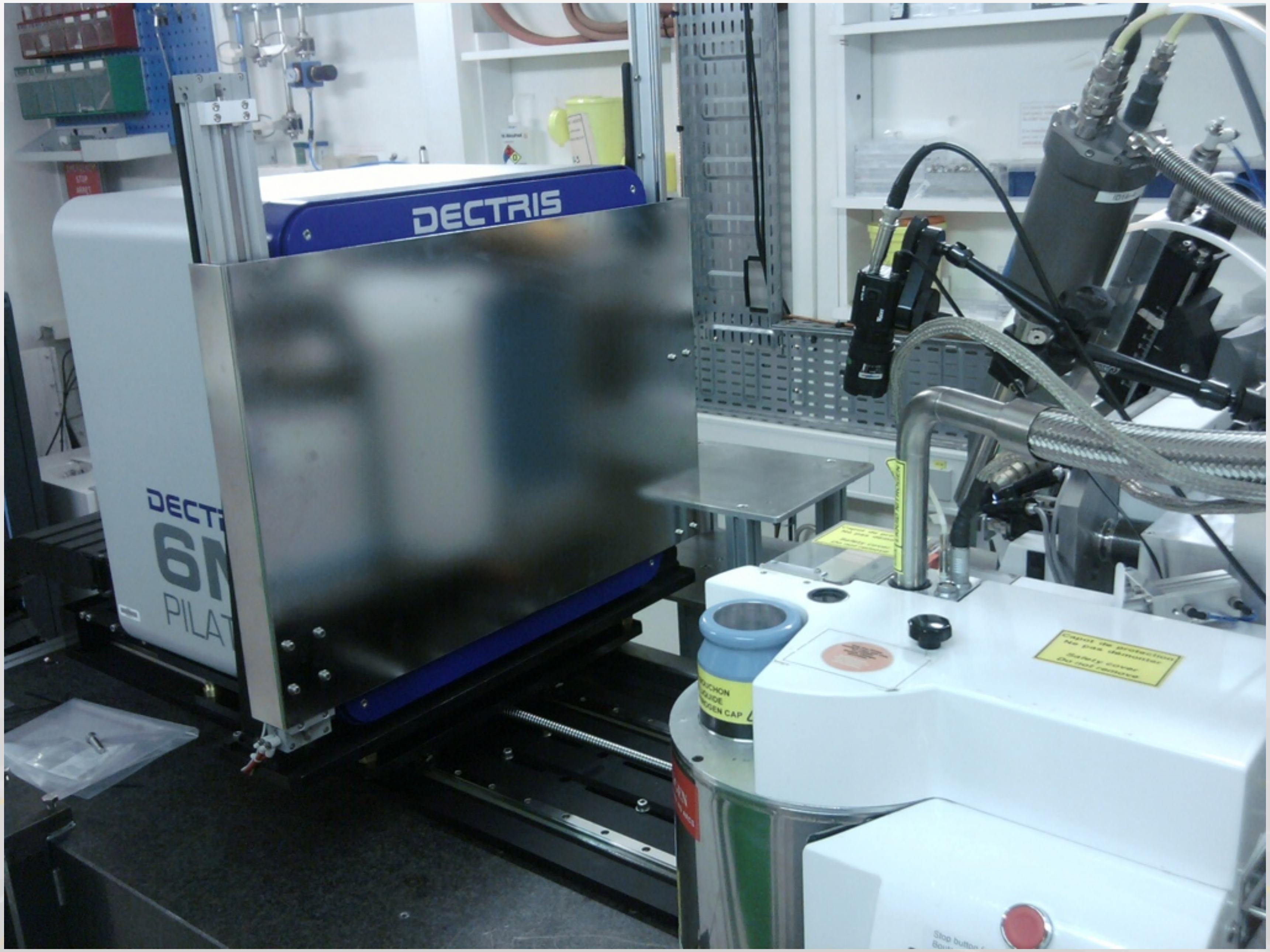






1. **Minikappa**
   1.1. Optimal orientation of the crystal
   1.2. Change orientation of the crystal (Friedel's pair on same frame)
2. **Microbeam**
   2.1. Best spot of the crystal
   2.2. Collect from different zone of the crystal
3. **Pixel detector**
   3.1. Fast readout - many frames collected in a few minutes
   3.2. No readout noise - great signal-to-noise
   3.3. Great data quality with fine slicing
   3.4. Shutterless data collection

Pilatus



100%QE at long wavelength

12hz frame rate

2ms readout time

Zero background noise

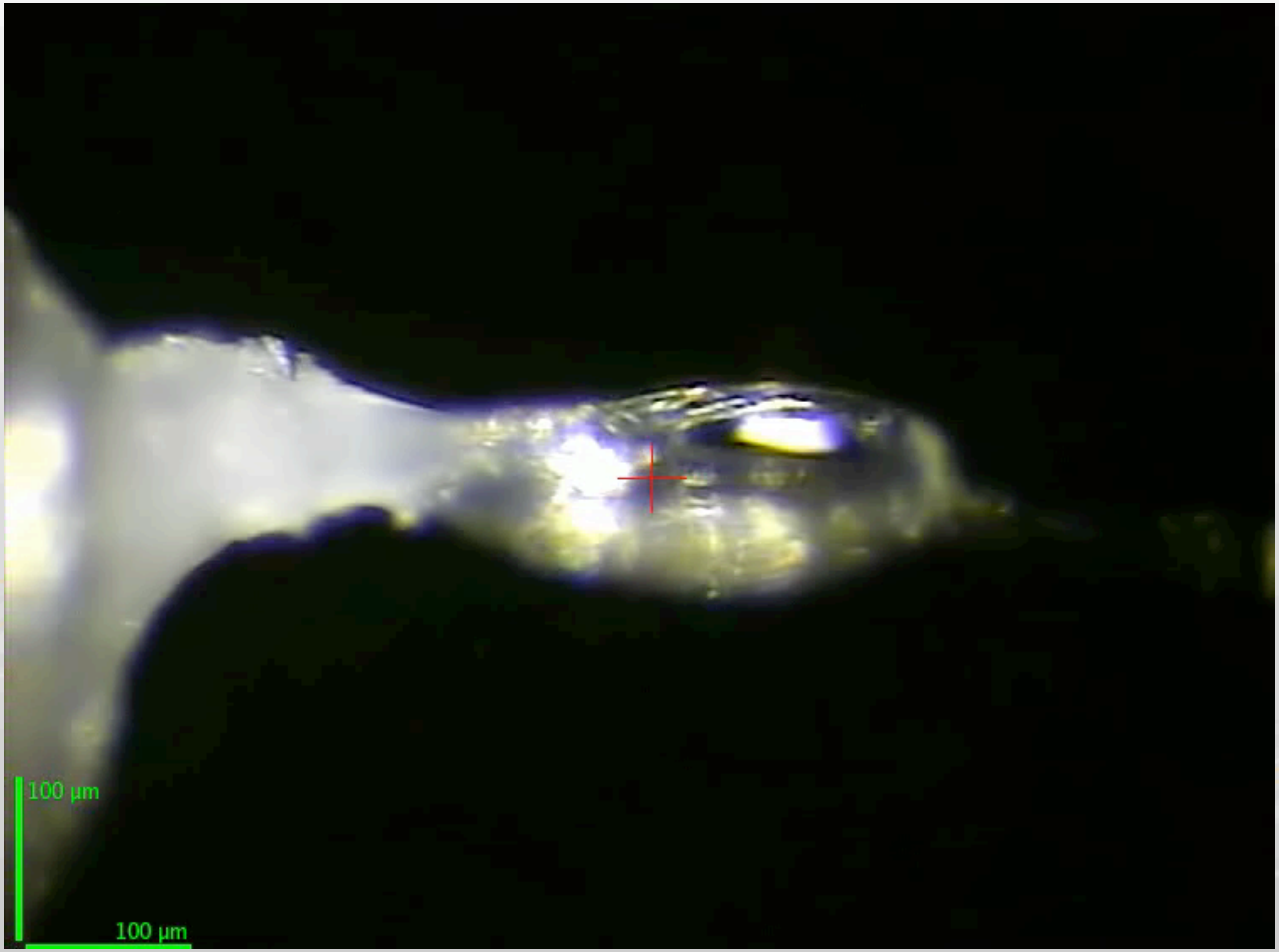
Zero point spread function

20bit dynamic range

typical dataset in less than 2 minutes

4D scans

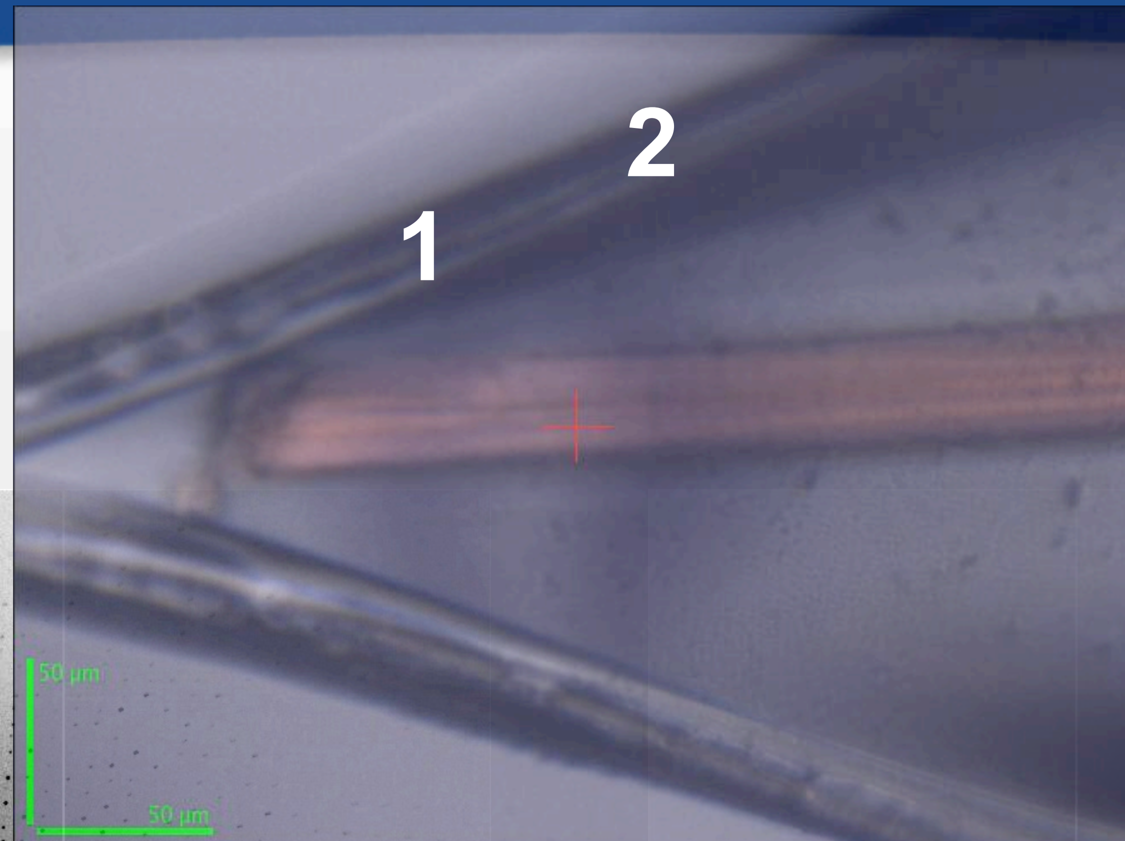
Fast readout and PMAC control permit to develop novel tasks and applications



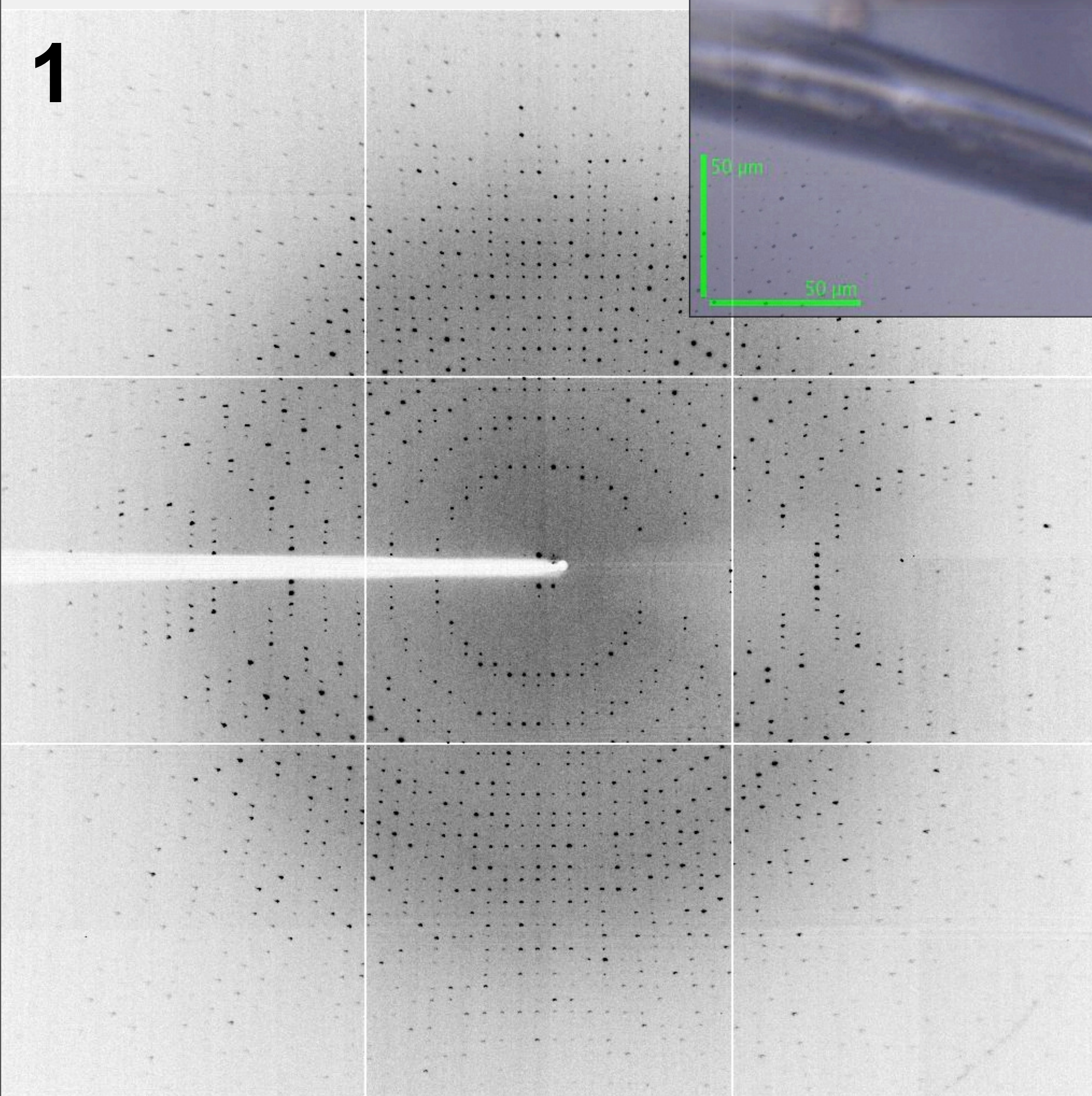
A good example

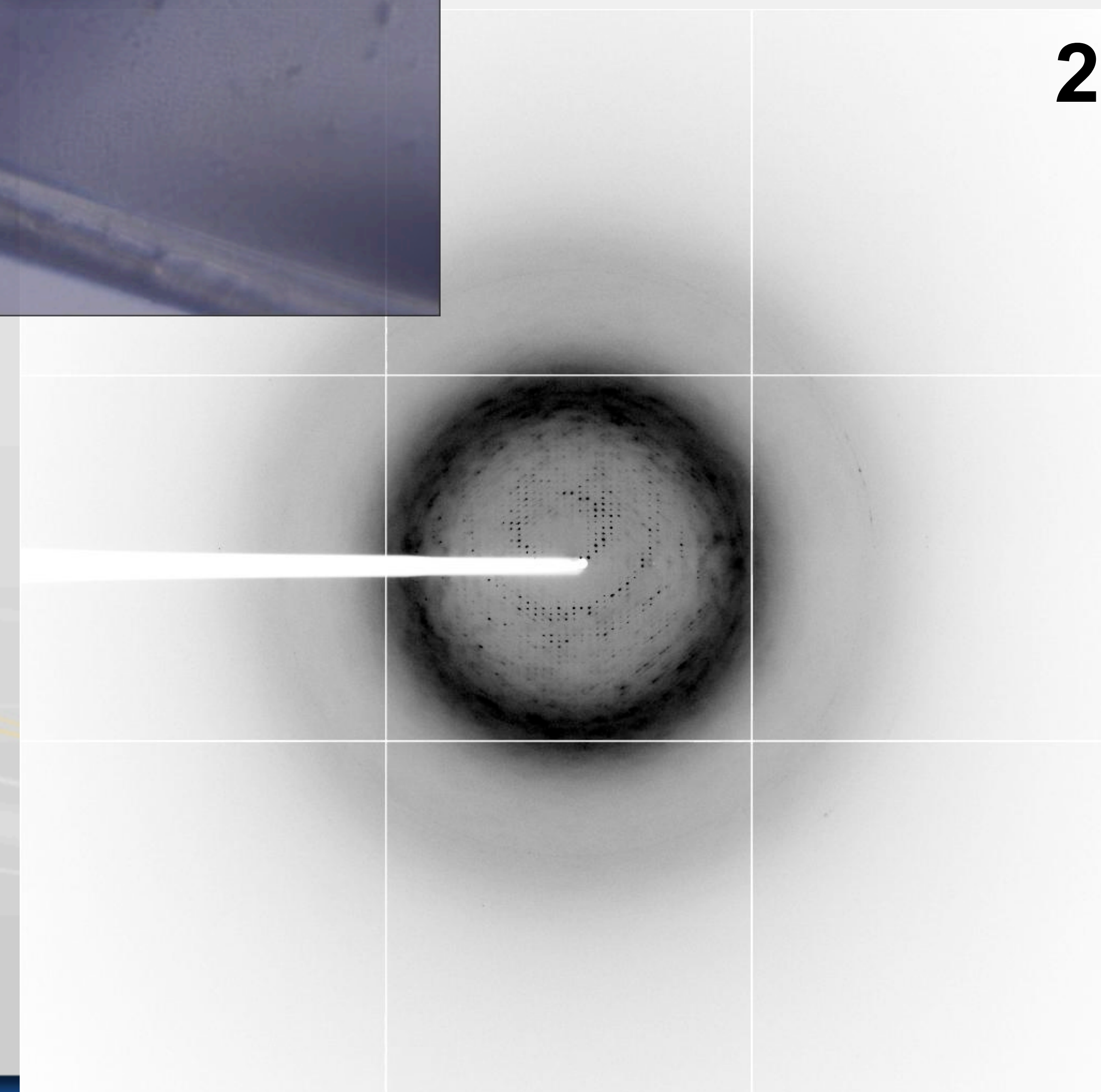
European Synchrotron Radiation Facility

4 Iron in 1180 residues, but also 16 Cys and 28 Met



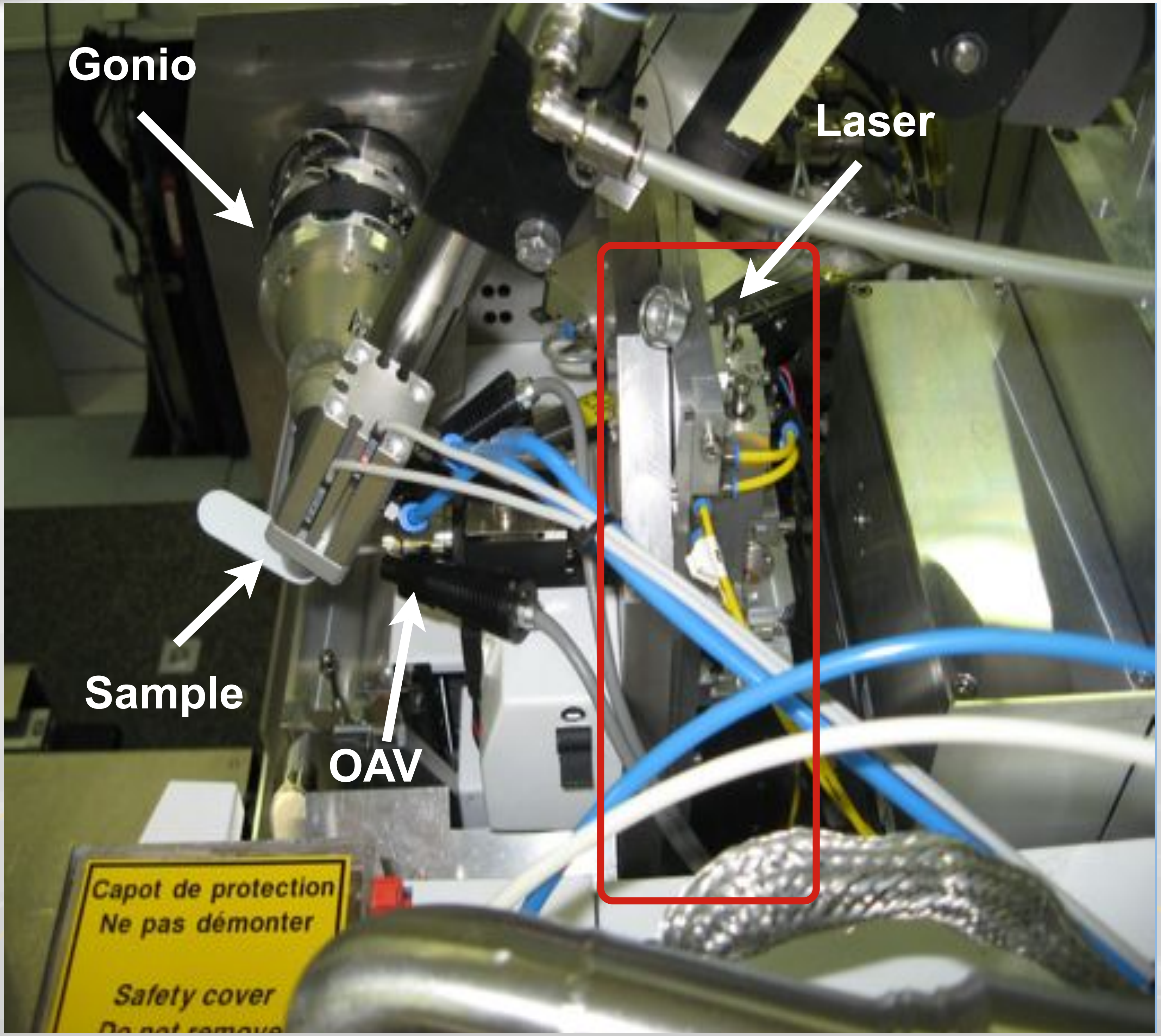
Long wavelength data, why not?

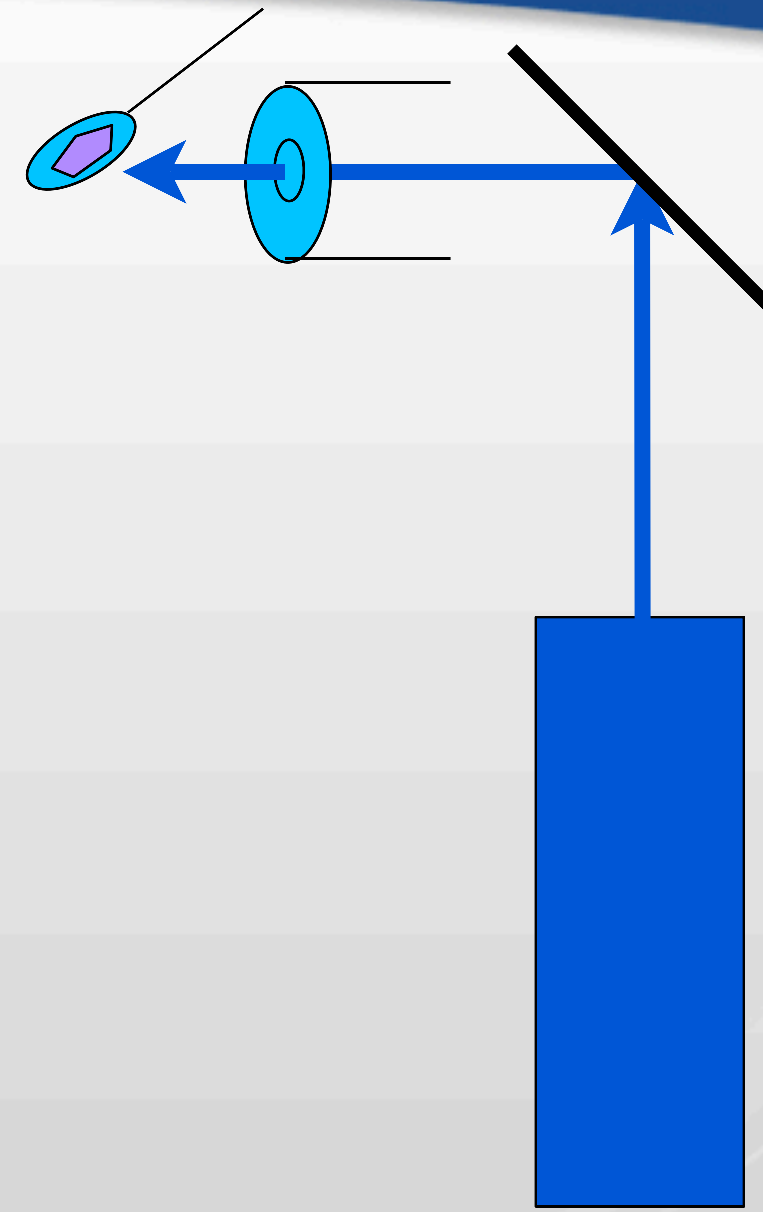




UV-RIP combined with S-SAD

UV laser on ID23EH1





Single isomorphous replacement phasing of selenomethionine-containing proteins using UV-induced radiation damage

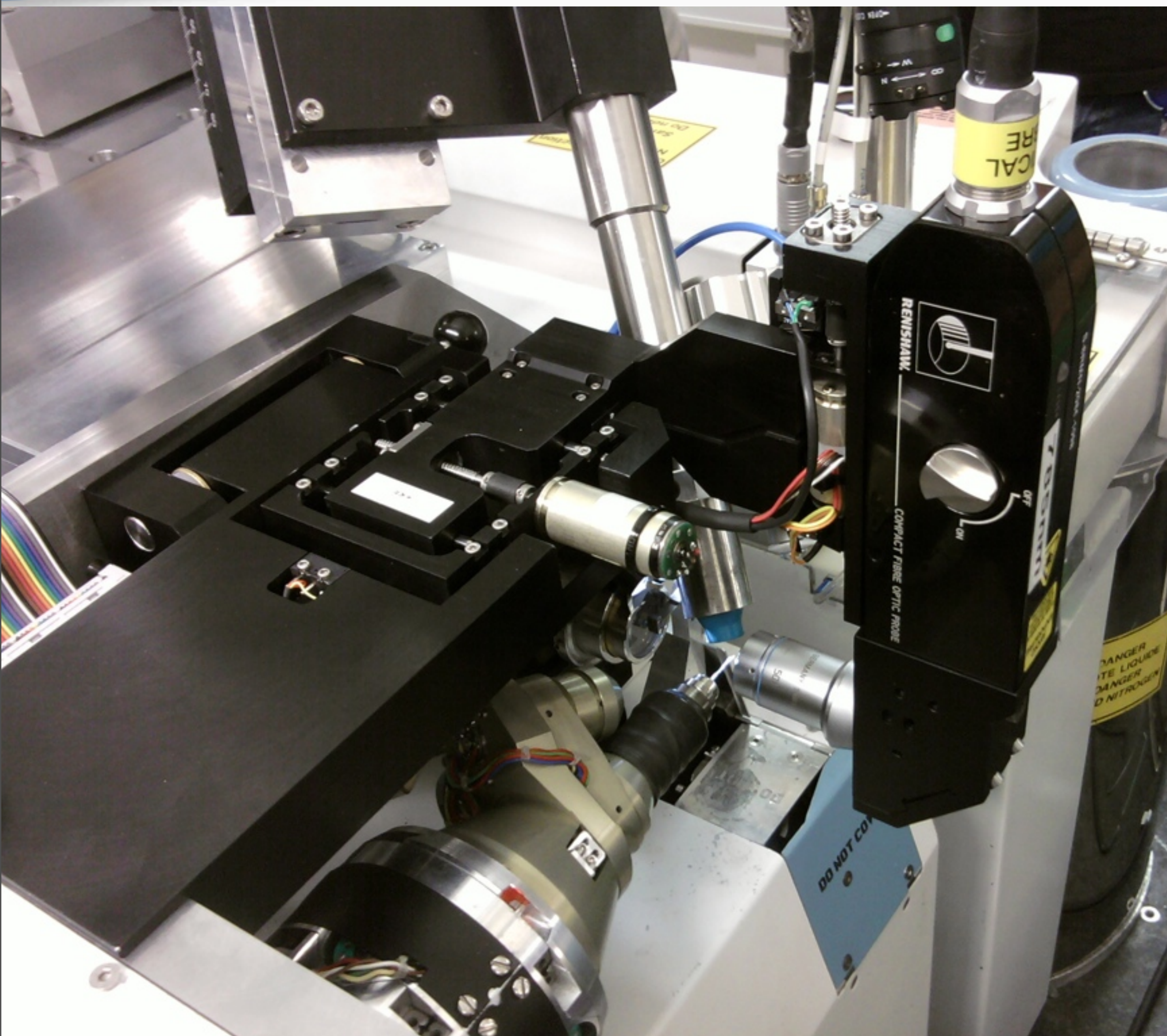
Santosh Panjikar,[a]* Hubert Mayerhofer,[a] Paul A. Tucker,[a] Jochen Mueller-Dieckmann[a] and Daniele de Sanctis[b]

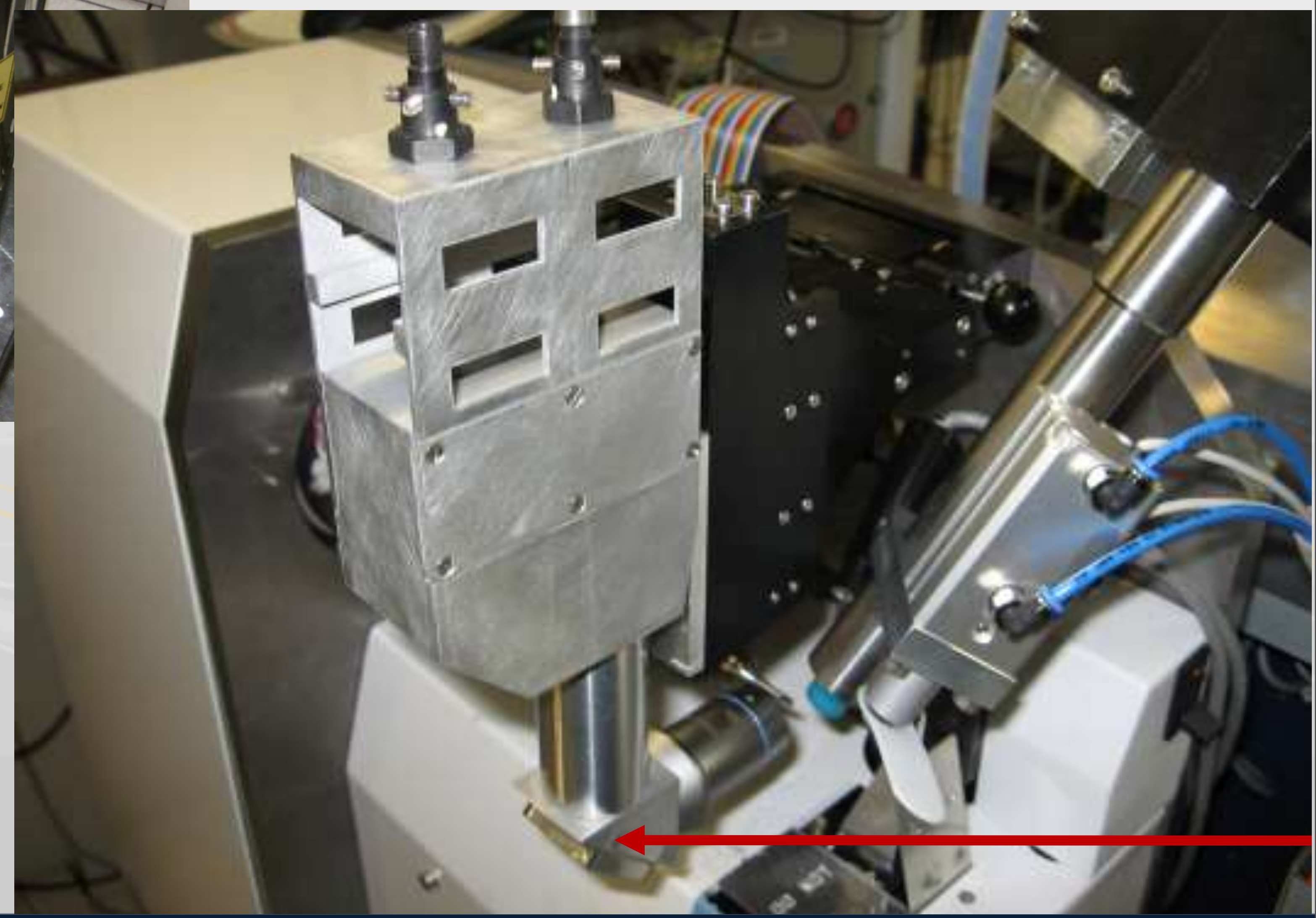
The most commonly used heavy-atom derivative, selenium, requires the use of a tunable beamline to access the Se *K* edge for experimental phasing using anomalous diffraction methods, whereas X-ray diffraction experiments for selenium-specific ultraviolet radiation-damage-induced phasing can be per-

Received 15 J
Accepted 21

ID29S on ID29

New multipurpose motorized support for **Raman**, **UV-RIP**, **Fluorescence**





Raman - follow disulfide breakage

Ways & Means

Raman-Assisted Crystallography Suggests a Mechanism of X-Ray-Induced Disulfide Radical Formation and Reparation

Philippe Carpentier[1], Antoine Royant[2, 3], Martin Weik[2], Dominique Bourgeois[1]

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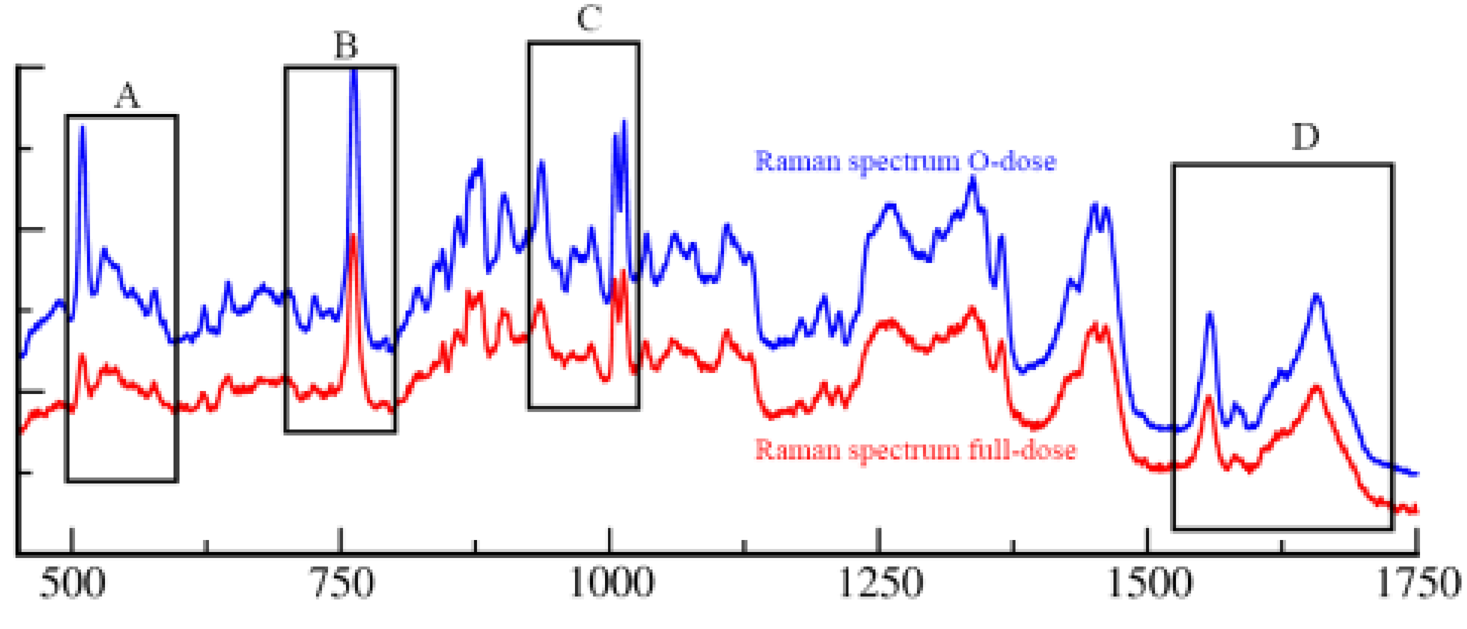
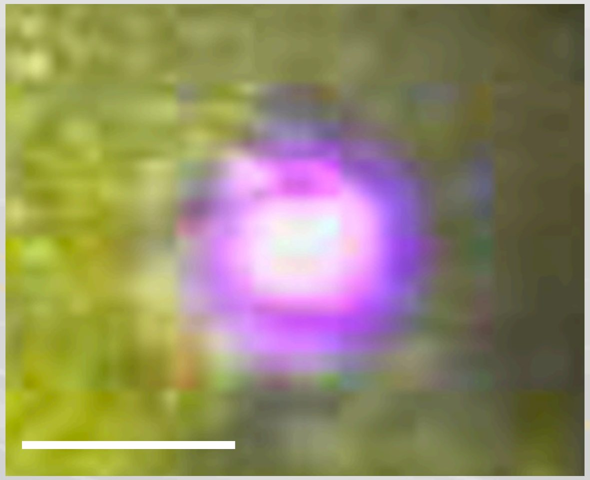
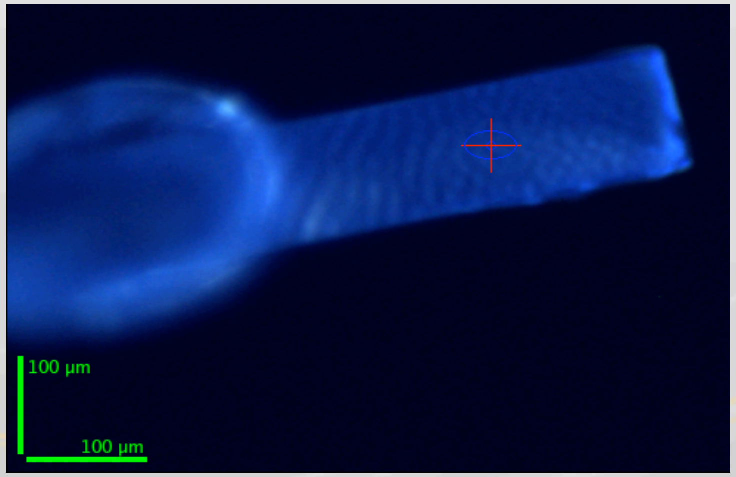
[2] Laboratoire de Biophysique Moléculaire, IBS, Institut de Biologie Structurale Jean-Pierre Ebel, CEA; CNRS; Université Joseph Fourier, 41 rue Jules Horowitz, F-38027 Grenoble, France

[3] European Synchrotron Radiation Facility, 6 Rue Jules Horowitz, BP 220, 38043 Grenoble Cedex, France



Irradiate with a Laser on a spot crystal





Thank you for your attention