

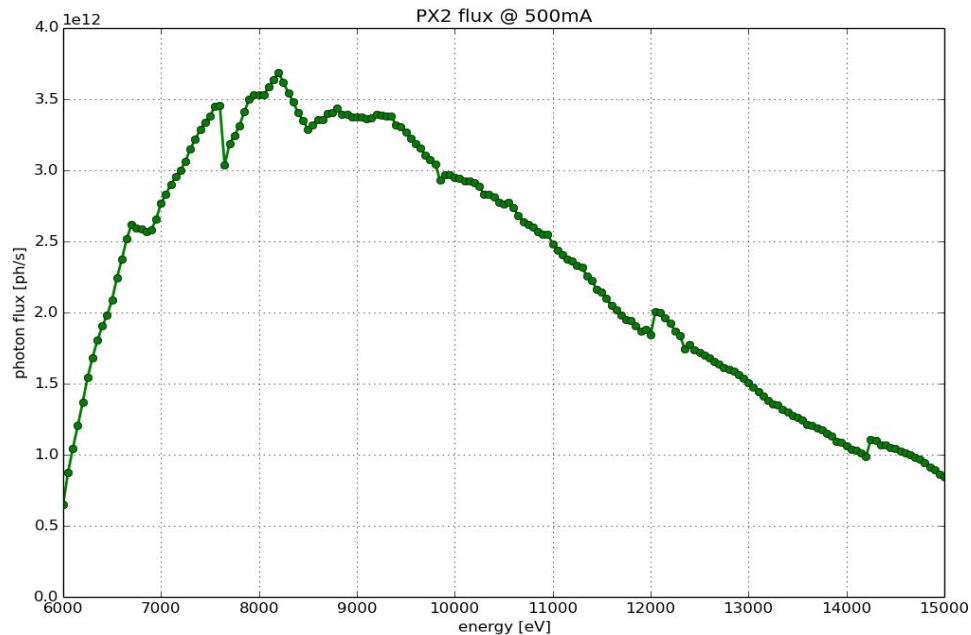
Towards systematic dosimetry on SOLEIL's Proxima 2A beamline

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Proxima 2A at SOLEIL

- 10x5 μm beam size (KB focusing)
- 3.6e12 ph/s @ 8.1keV
 - Tunable 6 - 18 keV
- MD2 goniometer with kappa head
- Eiger X 9M detector
- CATS sample changer
- 10k samples per year

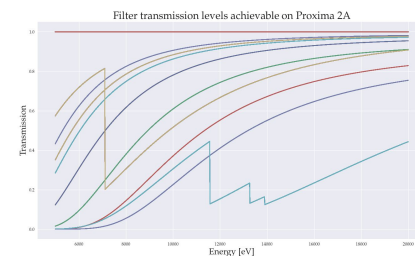
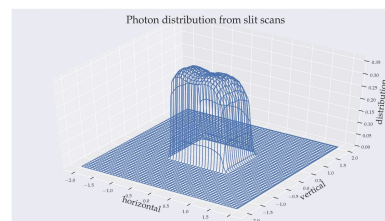
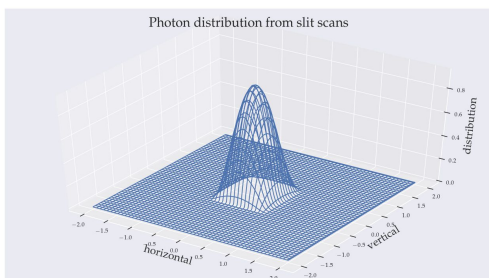
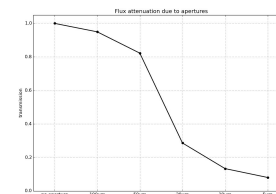
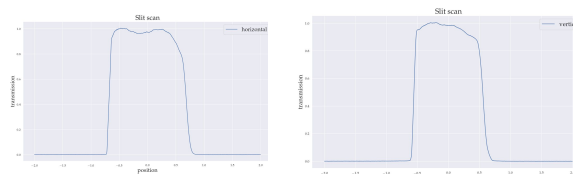
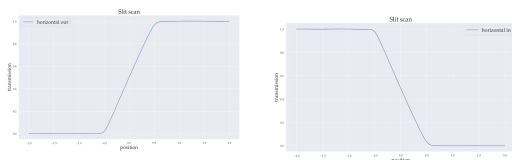
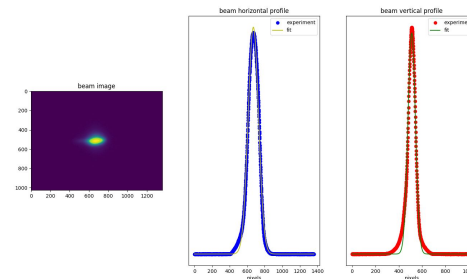


Motivation: look at very MX experiment as a radiation damage study

- Dose is the fundamental variable we worry about
- Key parameters determining the dose sample will receive
 - beam -- shape, intensity, energy
 - crystal -- shape, composition
 - sample environment -- shape, composition
- In the following I show how far we have been able to go along those fundamental directions

Beam properties

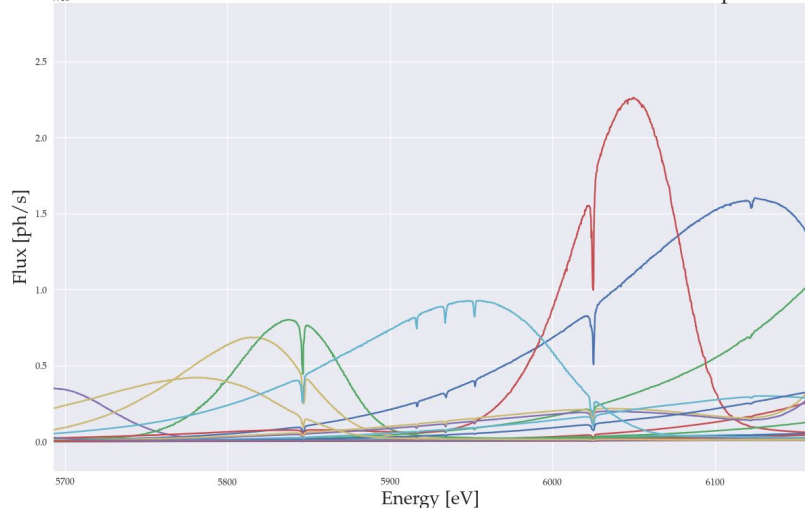
- AXUV 100 calibrated diode at sample position
- High resolution X-ray camera + On axis microscope
 - influence of beamline components on flux at sample
 - slits, filters, apertures, position monitors and monochromator



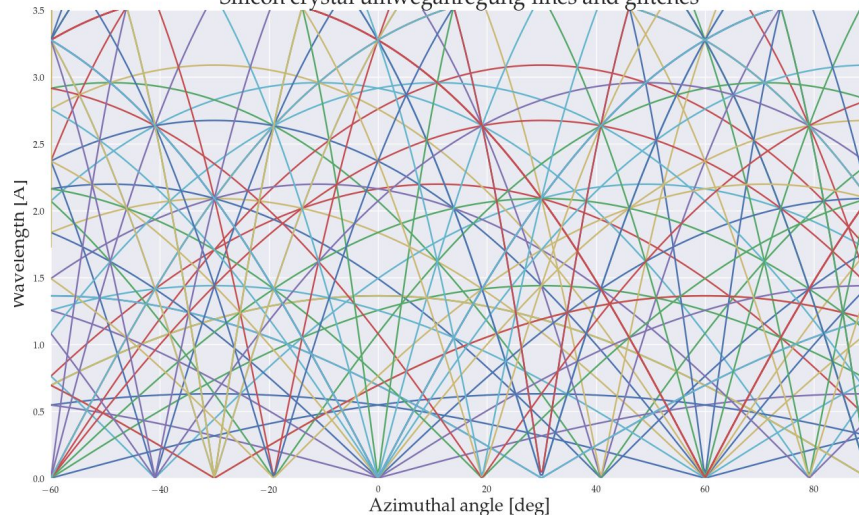
Better look at the monochromator

- Beware of monochromator crystal double diffraction and glitches
 - can be significant at specific energies

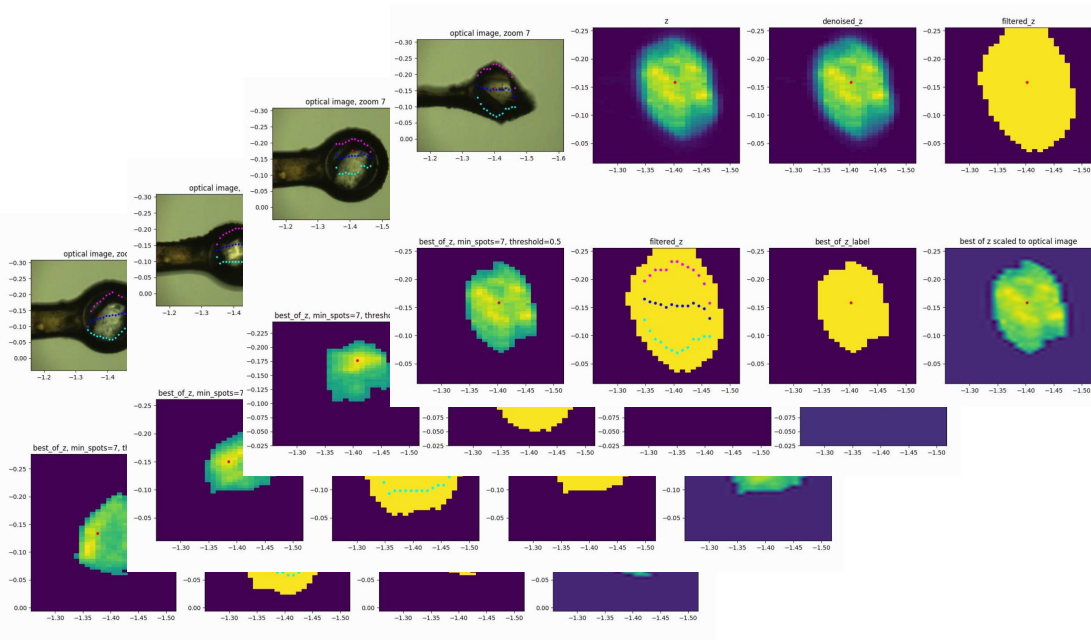
Monochromator Double Diffraction and Glitches Effect on Flux at Sample Position



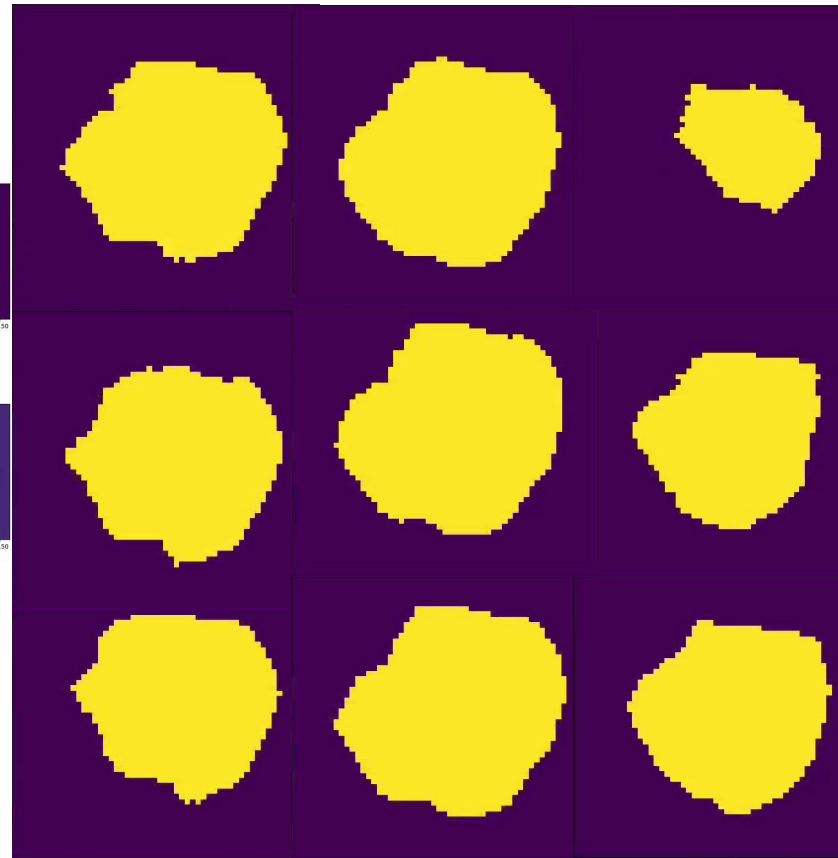
Silicon crystal umweganregung lines and glitches



Reconstructing crystal shape



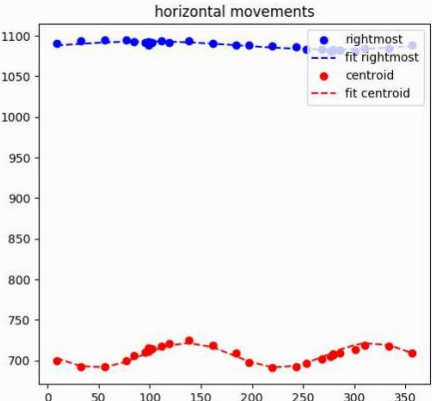
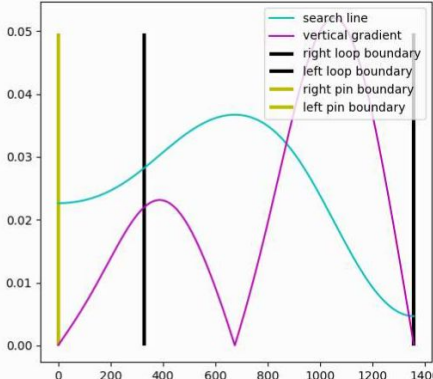
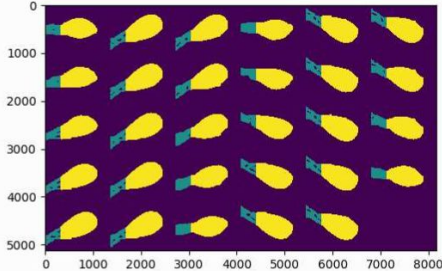
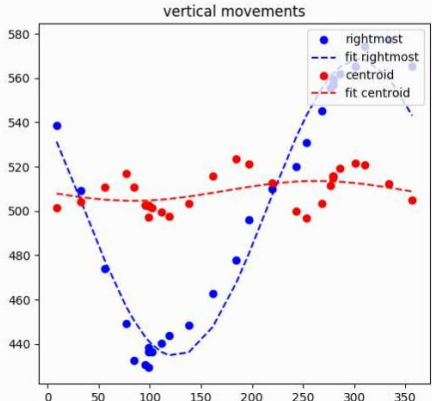
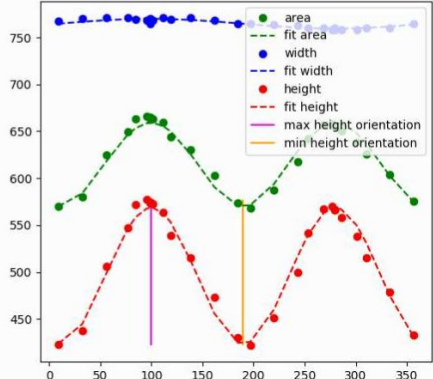
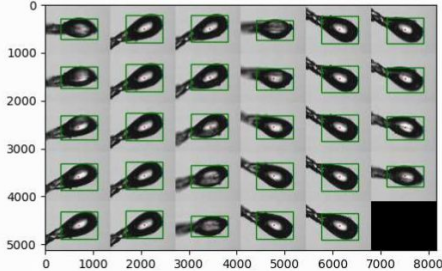
raster scans at four different orientations



reconstructed crystal shape along rotational axis

Reconstructing shape of sample environment

segmenting optical images -- optical based volume reconstruction



Outlook

- sample shape from optical images alone
 - premis: reconstructing sample shape purely from optical images is possible if sample is embedded in transparent medium
 - crystal will be tricky because of refraction -- needs to be taken into account
 - segment out support, mother liquor and crystal -- enhancing current pixel wise segmentation
- introducing dose as an experimental parameter?
 - warning of possibly dangerous combination of parameters

The dose (DWD) in the widget comes from RADDPOSE-3D with parameters for 30um cuboid lysosyme crystal with no heavy metals

Sample: 1:1

Standard Collection

Acquisition

Oscillation start (°):	<input type="text" value="0"/>	Range per frame (°):	<input type="text" value="0.1"/>
Number of images:	<input type="text" value="3600"/>	Total range (°):	<input type="text" value="360.0"/>
First image:	<input type="text" value="1"/>	Allowed range:	<input type="button" value="Full range"/>
Exposure time (s):	<input type="text" value="1"/>	Detector mode:	<input type="text" value="9M"/>
Kappa (°):	<input type="text" value="0"/>	Phi (°):	<input type="text" value="0"/>
Energy (keV):	<input type="text" value="12.65"/>	<input type="checkbox"/> MAD	<input type="text" value="ip: -"/>
Resolution (Å):	<input type="text" value="1.729"/>	Detector distance (mm):	<input type="text" value="180"/>
Transmission (%):	<input type="text" value="20"/>	Flux (ph/s):	<input type="text" value="8.25e+09"/>
<input checked="" type="checkbox"/> Shutterless		Estimated dose (MGy):	<input type="text" value="3.012"/>

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Number of images:	<input type="text" value="3600"/>	Total range (°):	<input type="text" value="360.0"/>
First image:	<input type="text" value="1"/>	Allowed range:	<input type="text" value="Full range"/>
Exposure time (s):	<input type="text" value="3"/>	Detector mode:	<input type="text" value="9M"/>
Kappa (°):	<input type="text" value="0"/>	Phi (°):	<input type="text" value="0"/>
Energy (keV):	<input type="text" value="12.65"/>	<input type="checkbox"/> MAD	<input type="text" value="ip: -"/>
Resolution (Å):	<input type="text" value="1.729"/>	Detector distance (mm):	<input type="text" value="180"/>
Transmission (%):	<input type="text" value="20"/>	Flux (ph/s):	<input type="text" value="8.25e+09"/>
<input checked="" type="checkbox"/> Shutterless		Estimated dose (MGy):	<input type="text" value="9.037"/>

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Standard Collection

Acquisition

Oscillation start (°):	<input type="text" value="0"/>	Range per frame (°):	<input type="text" value="0.1"/>
Number of images:	<input type="text" value="3600"/>	Total range (°):	<input type="text" value="360.0"/>
First image:	<input type="text" value="1"/>	Allowed range:	<input type="button" value="Full range"/>
Exposure time (s):	<input type="text" value="7"/>	Detector mode:	<input type="text" value="9M"/> ▾
Kappa (°):	<input type="text" value="0"/>	Phi (°):	<input type="text" value="0"/>
Energy (keV):	<input type="text" value="12.65"/>	<input type="checkbox"/> MAD	<input type="text" value="ip: -"/> ▾
Resolution (Å):	<input type="text" value="1.729"/>	Detector distance (mm):	<input type="text" value="180"/>
Transmission (%):	<input type="text" value="20"/>	Flux (ph/s):	<input type="text" value="8.25e+09"/>
<input checked="" type="checkbox"/> Shutterless		Estimated dose (MGy):	<input type="text" value="21.086"/>