Optimizing the Dose Distribution with Small Beams

Serane Sirigu, Pierre Legrand, William Shepard and Martin Savko

Synchrotron SOLEIL, L'Orme des Merisiers, Saint Aubin, 91192 Gif sur Yvette, France

*Author Email: savko@synchrotron-soleil.fr*

Introduction

The fundamental variable governing radiation induced changes in crystals of biological macromolecules is the dose -- energy absorbed by the crystal during its lifetime. Ideally we should be able to control for it when designing the experiment. To do so we need to have a pretty good idea of the properties of the probe (photon energy, shape, intensity) and those of the sample (shape, composition) and their relative movements during the experiment.

Reconstructing shape of sample environment

Series of optical sample images acquired over the rotational range of omega axis is used to determine key characteristics of the sample containing volume yielding
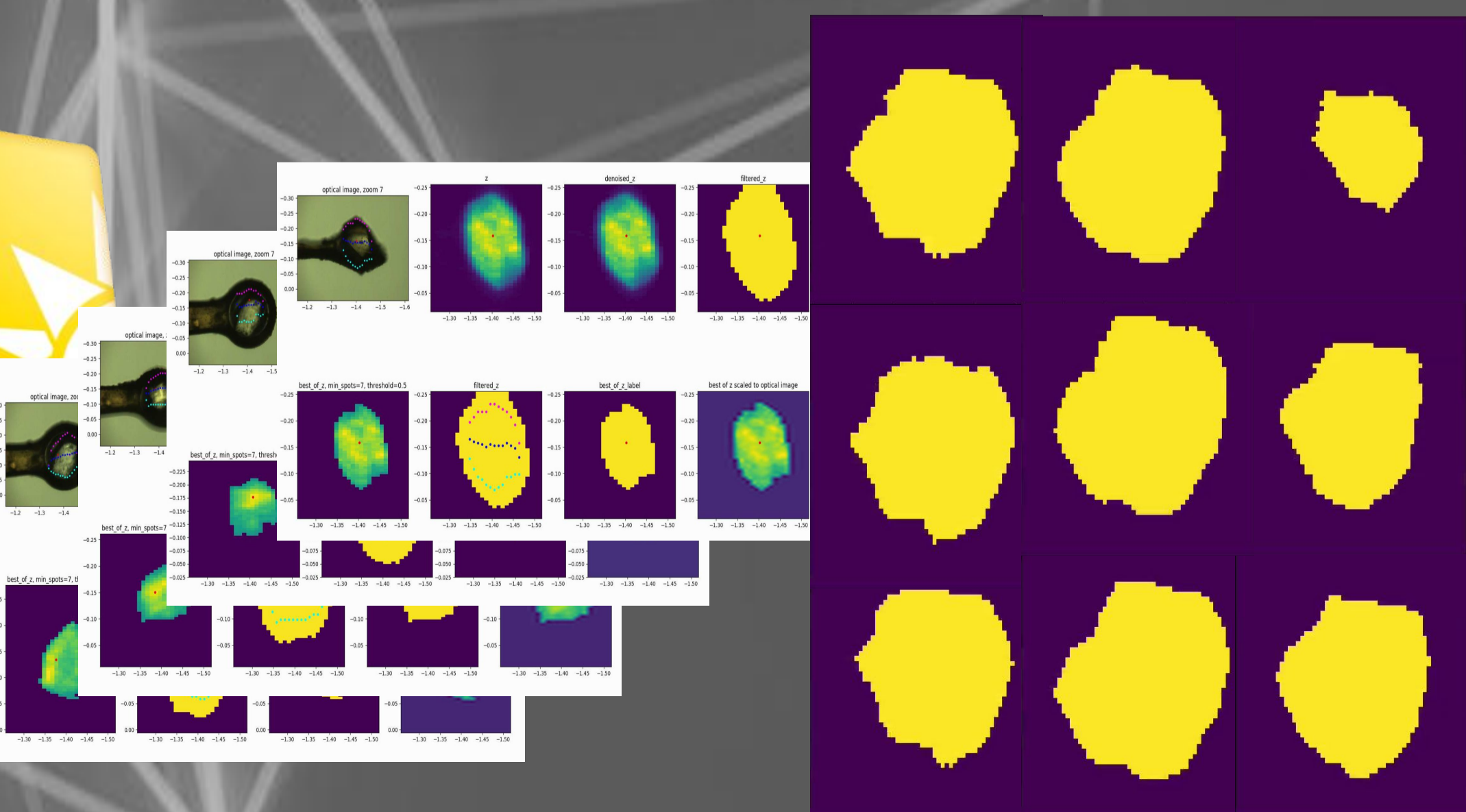
- loop bounding box at arbitrary orientation
- aligned center of the loop
- parameters of area to search with X-rays
- reconstructed volume enclosing the crystal
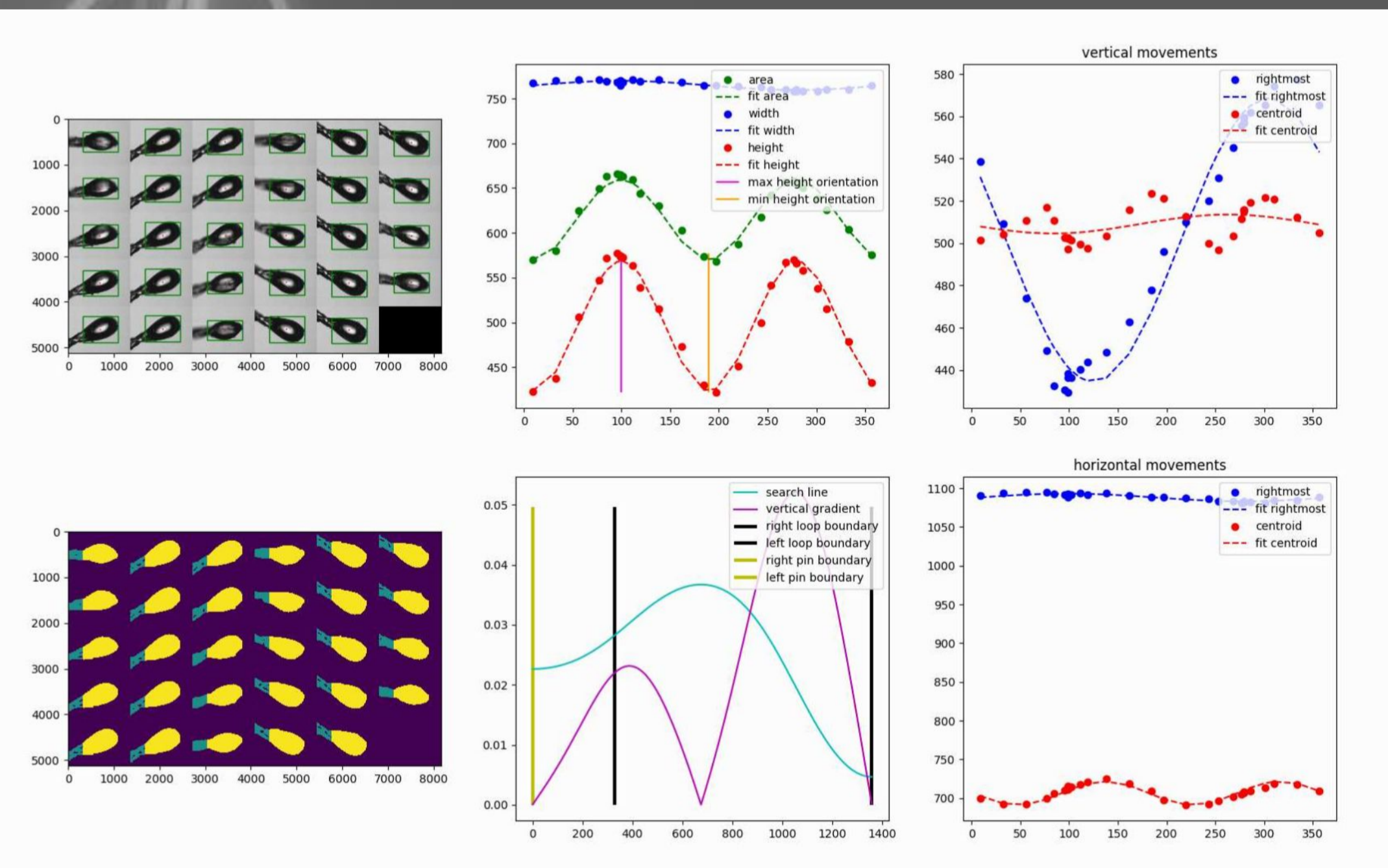
Reconstructing crystal shape

Find the zones that diffract:

- crystal size and shape
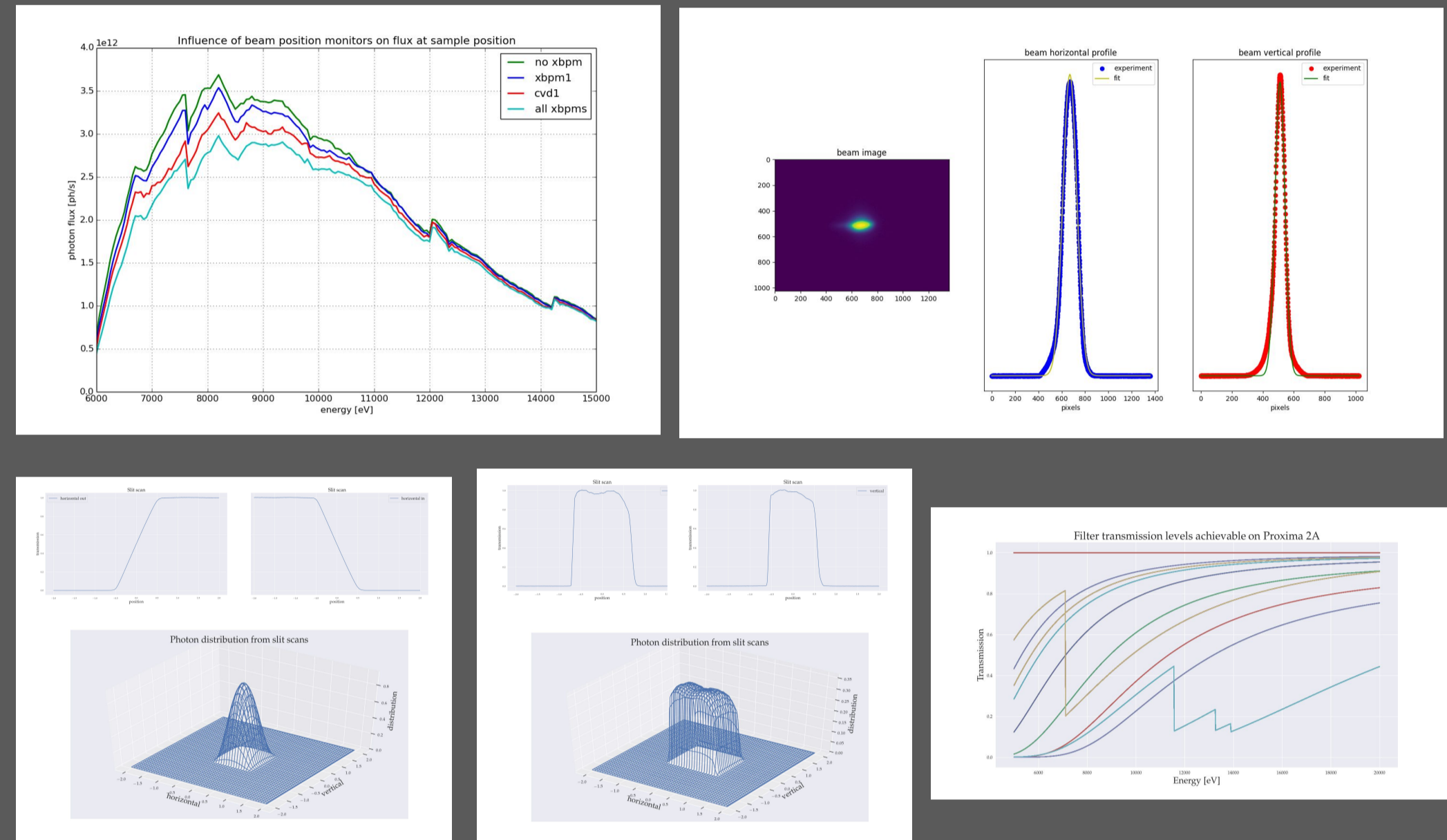- crystal quality and its variability
- crystal center curve model

raster scans at four orientations

reconstructed crystal shape along rotational axis
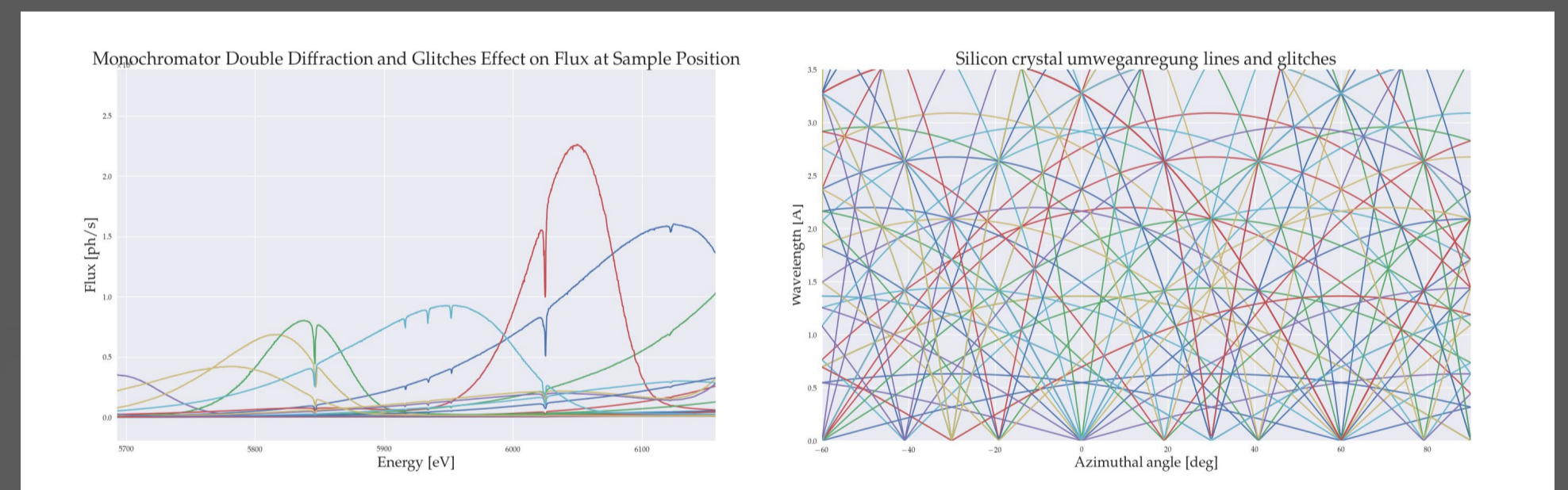
Controlling beam properties

The x-ray probe

- size
- profile
- intensity
- photon energy
- influence of beamline components on flux at sample
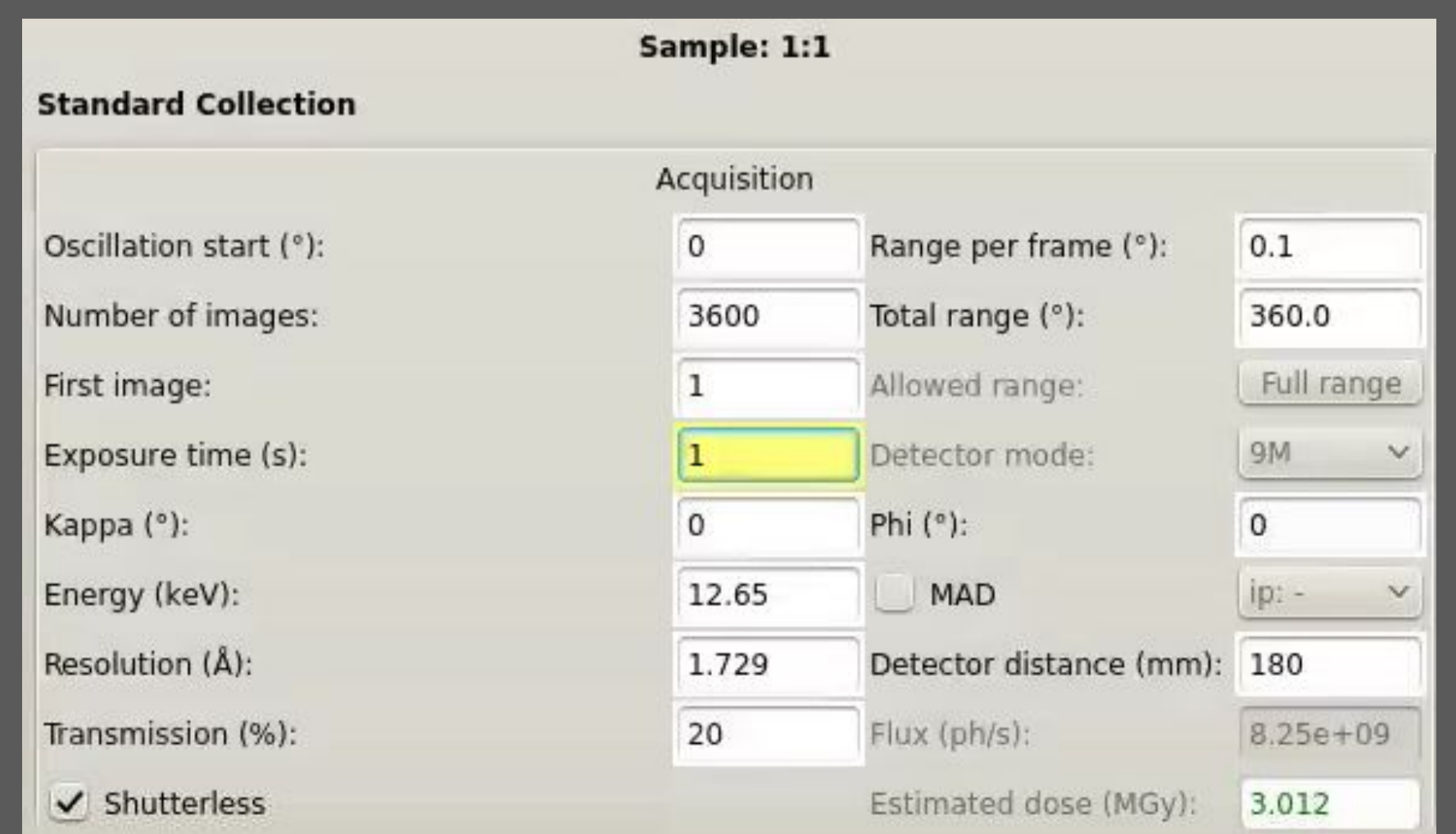- slits, filters, apertures, position monitors and monochromator

Better look at the monochromator

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

Outlook

- sample shape from optical images alone
  - premis: reconstructing crystal shape purely from optical images is possible if sample is embedded in transparent medium
  - segment out support, mother liquor and crystal -- enhancing current pixel wise segmentation
  - dose as an experimental parameter

Sample: 1:1			
Standard Collection			
	Acquisition		
Oscillation start (°):	0	Range per frame (°):	0.1
Number of images:	3600	Total range (°):	360.0
First image:	1	Allowed range:	Full range
Exposure time (s):	1	Detector mode:	9M
Kappa (°):	0	Phi (°):	0
Energy (keV):	12.65	MAD	ip: -
Resolution (Å):	1.729	Detector distance (mm):	180
Transmission (%):	20	Flux (ph/s):	8.25e+09
✓ Shutterless		Estimated dose (MGy):	3.012

acquisition widget with the dose field