LiX status

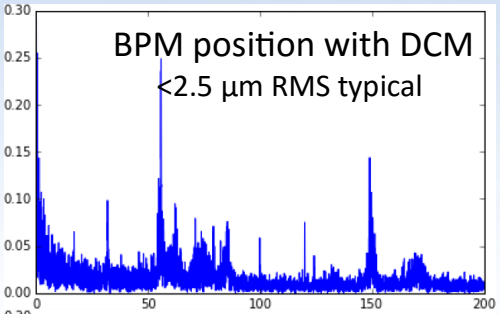
LSBR Advisory Meeting, Mar 28, 2017

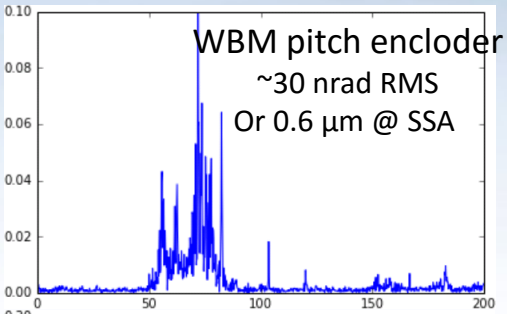
Progress since the last advisory meeting

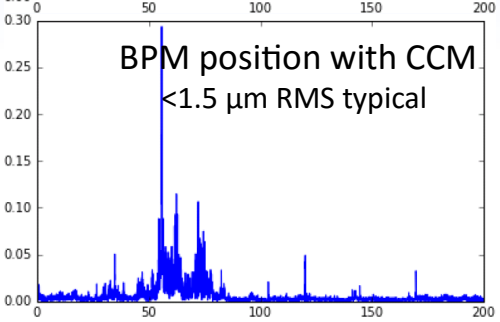
- Commissioning
  - Beamline components under control with CSS and Ophyd/Bluesky
  - Still finalizing the optics alignment routines
- Solution scattering
  - High throughput static measurements and in-line size exclusion chromatography available to users through rapid access
- Micro-beam diffraction
  - Routine measurements with 5-micron beam
  - Exploring data collection and analysis with several user groups

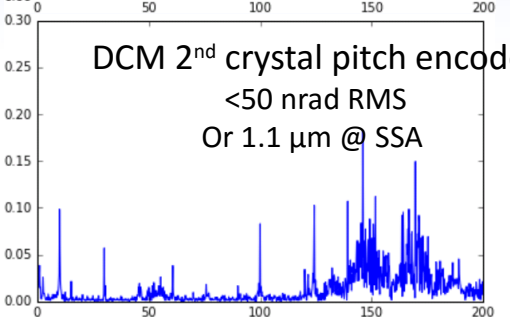
Some results from commissioning

Beam stability characterization



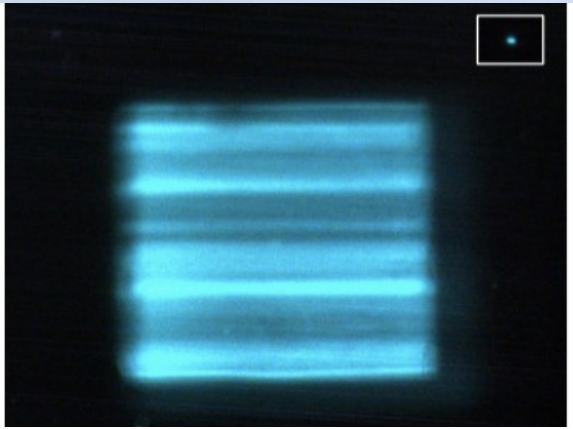






Fourier amplitude of beam position and encoder position in frequency domain (Hz).

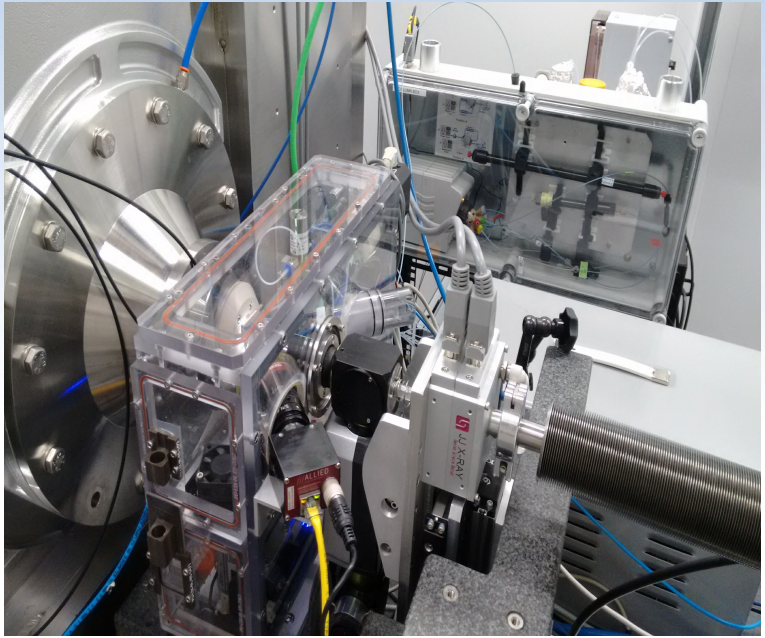
Secondary focusing optics commissioning

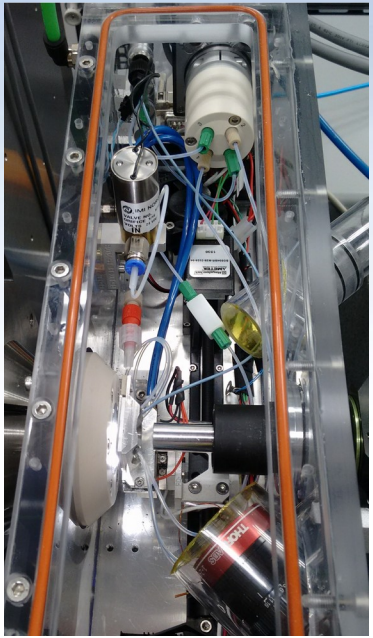


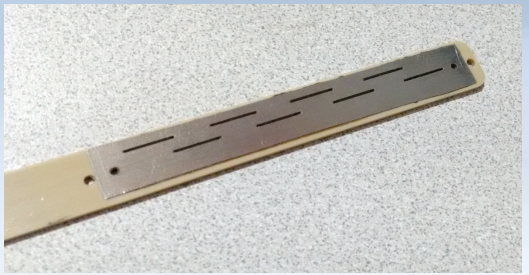
Beam observed during commissioning on a scintillator at the sample position through the on-axis microscope, without and with CRLs. The beam sizes are ~0.5mm and ~10 microns.

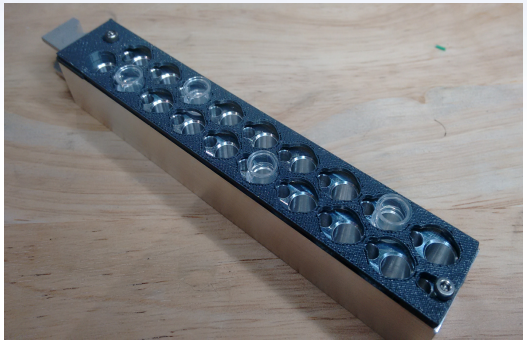
- Did enough to get experiments going; will continue to refine and automate routines for alignment and recovery

Solution scattering: the experimental module



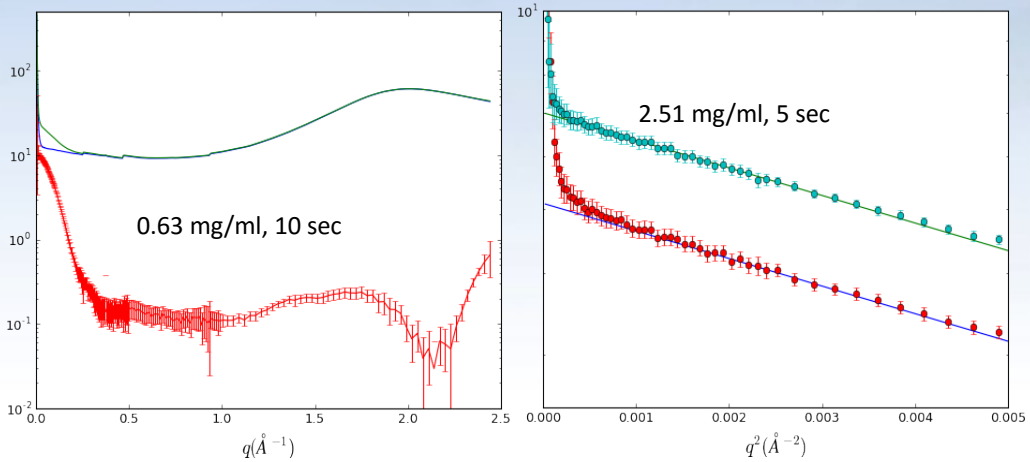




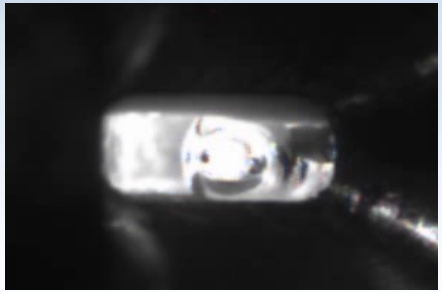


- Can accommodate different type of sample cells, in a helium environment
- HPLC system integrated into a rack; parked in close proximity to the solution scattering enclosure to reduce peak broadening; switch between static measurements and in-line SEC on demand

Pushing for lower sample volume and conc.



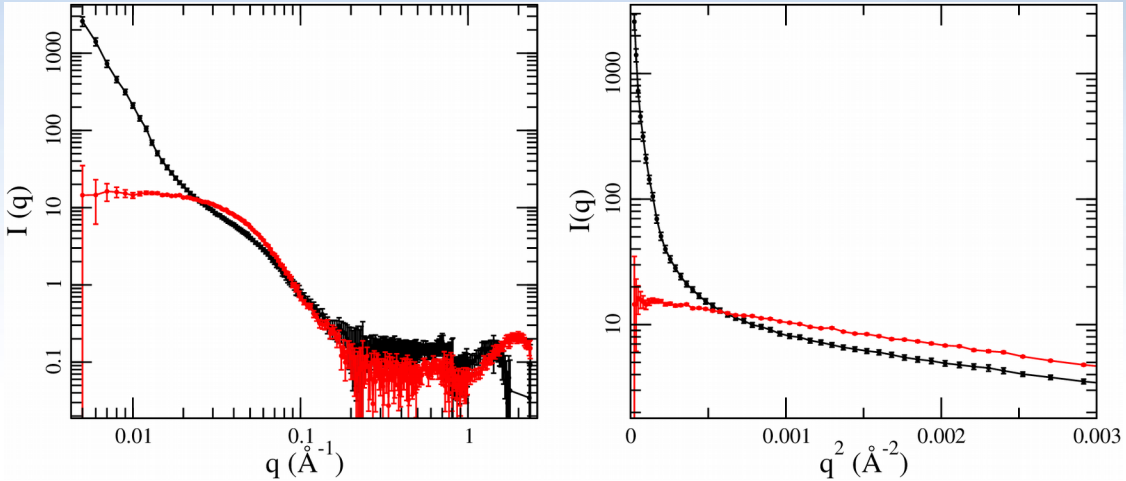
Scattering from Ribonuclease A (13.7 kDa) solutions collected during commissioning



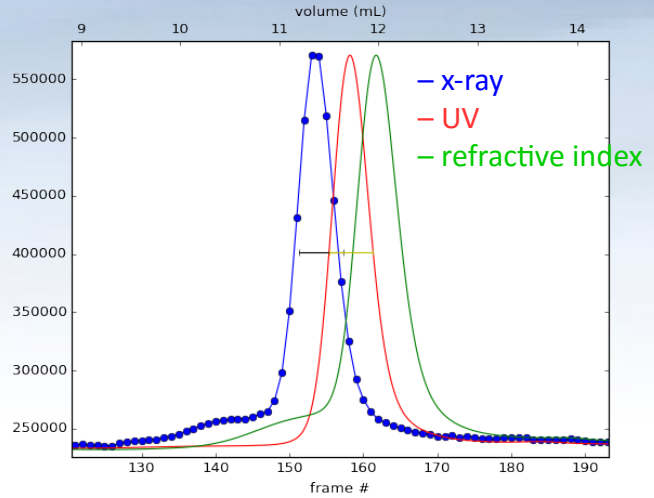
A solenoid valve has been installed for removing bubbles appearing in the HPLC channel of the flow-through cell

- ~50 µL per measurements, limited by radiation damage and reliability (issues with bubbles, unexpected delays in Bluesky)
- Continually iterating the cell design and data collection routine to improve reliability; to work on video-based data collection trigger

In-line size exclusion chromatography



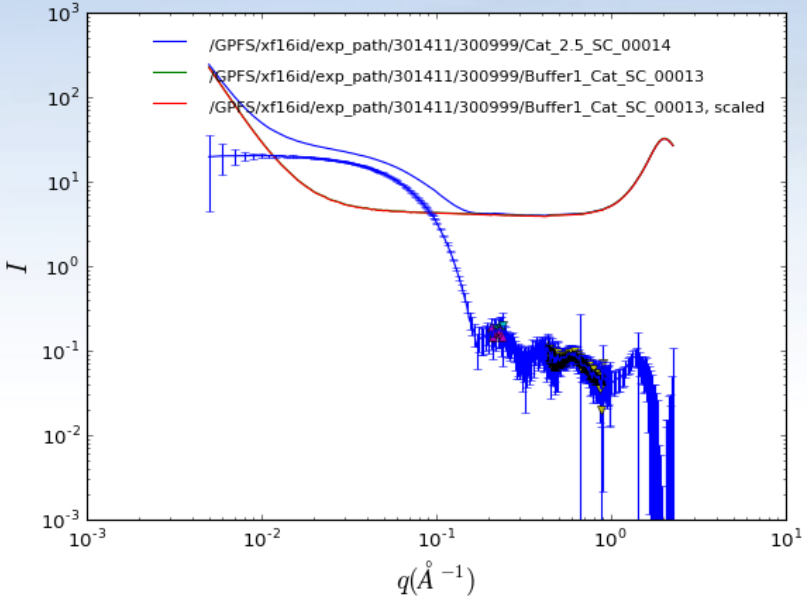
Data collected by Hubbard group (NYU) without and with in-line purification. The user was convinced to try out the purification system while at the beamline.



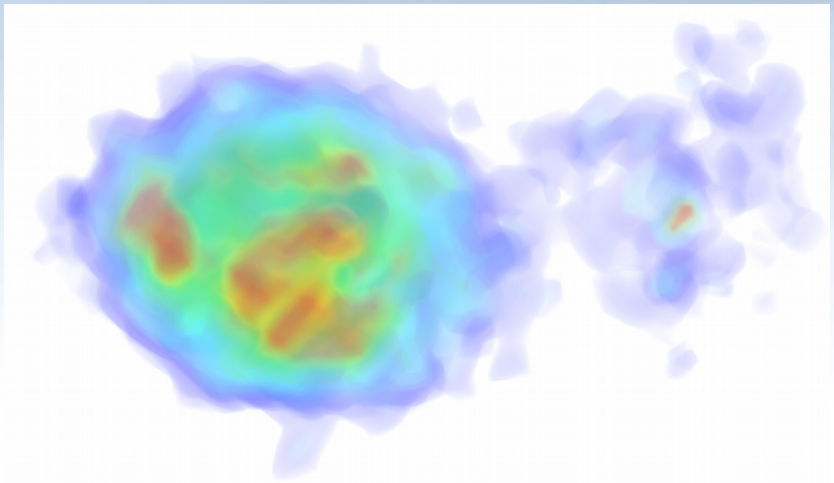
Data from beta-Amylase collected during recent calibration measurements

- In-line purification has been very helpful for our users; spent time characterizing the system (resolution limit, dilution factor, etc.) to help users better design their experiment
- Will work with BNL Computer Science Initiative to try to maximize information output from the data from x-ray, UV and refractive index detectors

Wide angle scattering



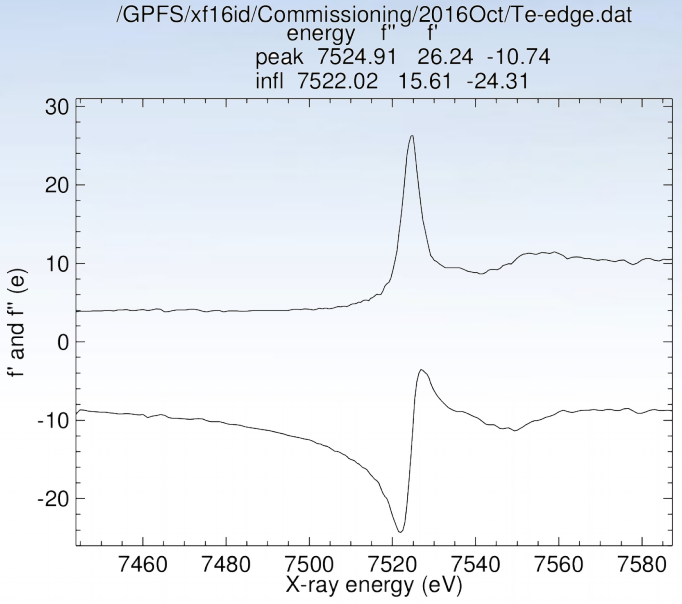
Data collected by Garcia-Diaz group (SBU)



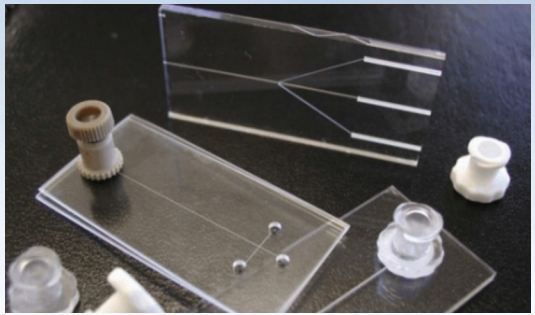
Model by Tom Grant (Hauptman-Woodward Institute) based on the data

- The intensity of the water peak is used as a reference for buffer subtraction; well-suited for automated data processing
- The scattering data always have a wide q-range (0.005-2.4 $Å^{-1}$); the high-q data may yield useful structural information

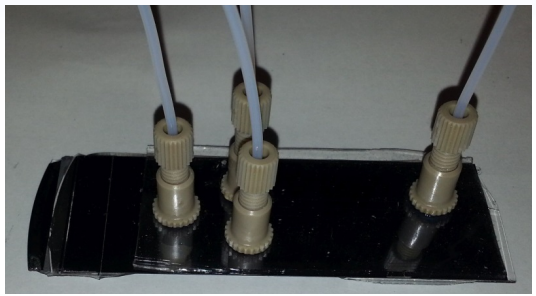
Other flavors of solution scattering



Chooch plot from data collected by Allen group (BU)



Flow mixer developed for time-resolved solution scattering by Osman Bilsel (U Mass). The flow channels are etched into quartz plates.

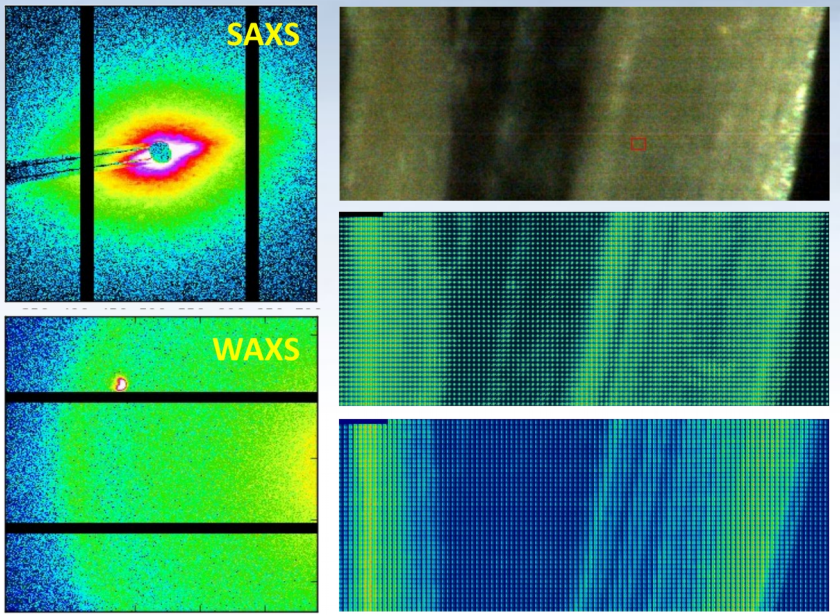


Flow mixer developed in house by Shirish being tested in the lab. The channels are etched in silicon and capped by sapphire windows.

- Collected anomalous scattering data; need to work on a data processing pipeline
- Developing a flow mixer in house for time-resolved measurements (Shirish); work with collaborators to make capability available to users sooner

Imaging based on scattering contrast

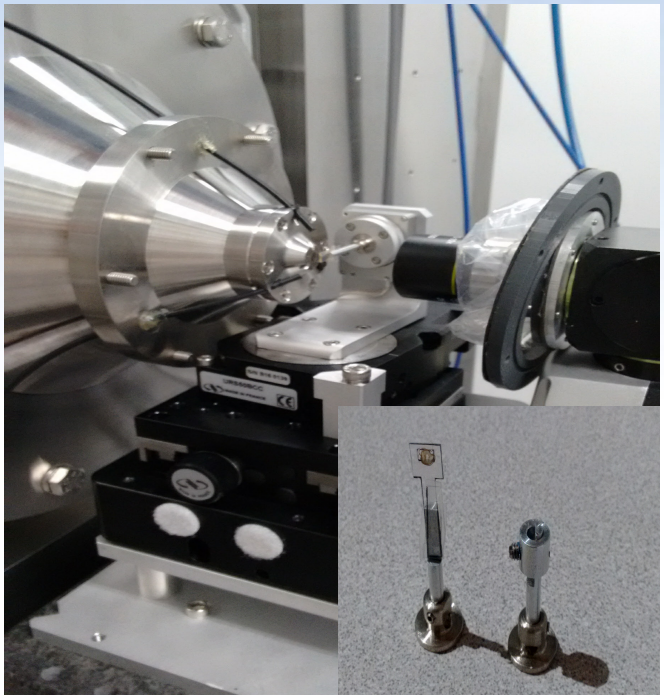
FOV ~ 0.5mm x 0.2mm

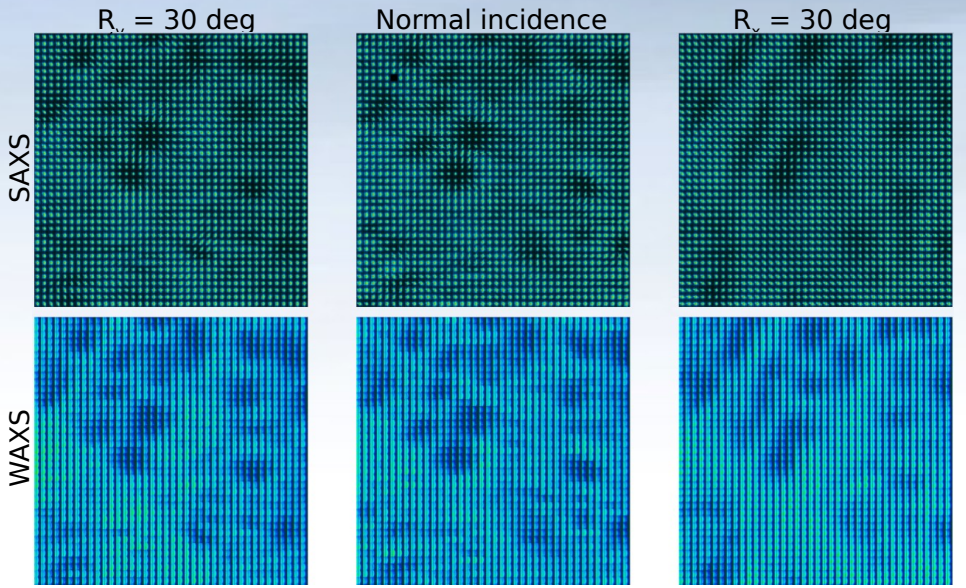


Individual and composite scattering patterns and the optical image from a plant section (L Makowski, NEU).

- Scattering contrast can reveal features not visible in other modes of microscopy
- Data analysis is non-trivial; working with the DAMA group and users to figure out how to process the data quickly and to yield scientifically useful information

Vectorial mapping



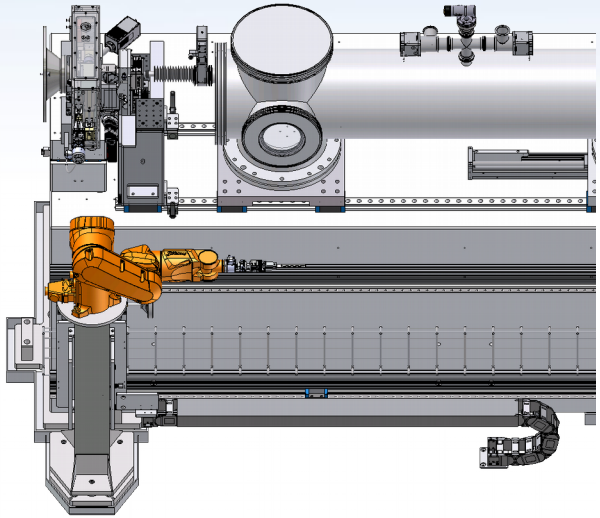


Scanning images of a plant section, measured at different sample orientations (CJ Liu, BNL). The images appear compressed in one direction and show different intensity variations due to the viewing angles .

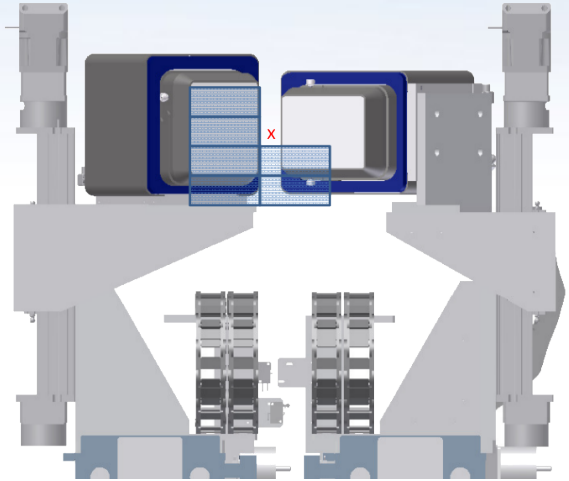
- When the sample contains periodic structures, the direction of the periodicity could be determined from how the scattering pattern changes with sample orientation

Future plans

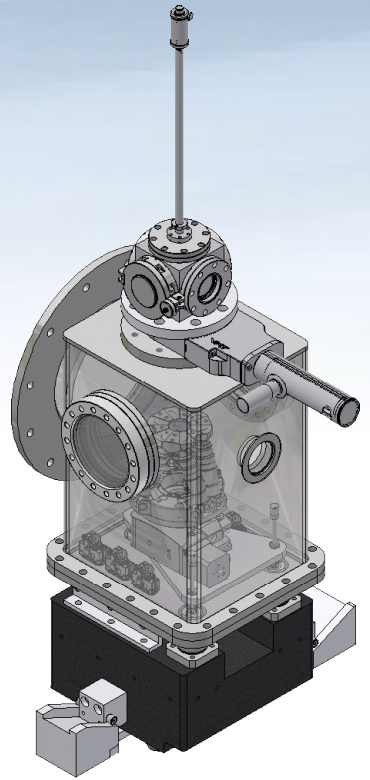
- Automation based on Staubli TX40 robot
- Upgrade of WAXS detector (have preliminary quote from Dectris)
- Helium environment for experiments at low energy



A 6-axis robot will manage samples for solution scattering for unattended automated measurements



An L-shaped WAXS detector to provide better azimuthal coverage in microbeam diffraction experiments



An experimental module for low-E or in-vacuum experiments

Challenges

- Software implementation/development/optimization
  - Automated optics optimization
  - Perform scans more quickly using BlueSky without delays
  - More intelligence in automated measurements
    - e.g. bubble removal, sample alignment in micro-beam mapping
  - Processing large data sets quickly
    - Make use of the GPU servers; more automation; interface with DAMA data browser
  - Graphical UIs for users
  - Automated data analysis
- Integration of hardware
  - TX40 robot
  - hexapod