Design, Construction and Commissioning of Two Highly Integrated Experimental stations for micro-focusing Macromolecular Crystallography (MX) Beamlines at NSLS-II

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We present the final engineering design and first commissioning results of two highly integrated experimental stations for the micro-focusing (FMX) and the highly automated (AMX) MX beamlines at the NSLS-II. These beamlines will support a broad range of biomedical structure determination methods from serial crystallography on micron-sized crystals, to structure determination of complexes in large unit cells. These experimental stations are completely designed and fabricated in-house to meet challenging requirements resulting from the small beam size of 1 µm and the extremely short working distance of only 190 mm from the beam exit window to the FMX focal spot.

The beam conditioning unit contains, within 140 mm, a beam position monitor, an attenuator, primary slits, an intensity monitor, a sub-millisecond shutter, and secondary slits. The diffractometers consist of an interchangeable high precision air bearing based main goniometer and a secondary goniometer for crystallization plates, both with a SOC of 100 nm on horizontal axes, an on-axis microscope with a customized reflective optics, x-ray fluorescence detector and dynamic beam shaping slits. Both these robotic end stations are integrated in a compact space on a granite machine bed with high modularity for future upgrades and extensions. Novel automation concepts are being implemented to increase the through-put of the cryogenic samples.

FMX and AMX scientific missions

Specialize and Complement	FMX will cover the micro-beam regime and AMX the mini-beam regime, yet both lines have complementary and overlapping capabilities
Vast numbers	AMX will support programs that require testing of vast numbers of specimens, e.g. studies of membrane proteins, and drug discovery explorations
Micro-crystals, serial crystallography	FMX will provide a micron sized beam and sample delivery and data processing to support efficient structure determination from micron sized crystals
Large unit cells	FMX and AMX will support structure determination of multi-component assemblies
Collect on all	High flux and short data collection times will make it possible to collect on every specimen, assisted by crystallographic decision making software
Remote	Remote data collection from home institutions

FMX

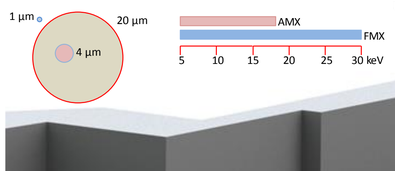
Energy range	5 – 30 keV
Wavelength range	0.4 – 2.5 Å
Flux at focus	~10^{13} ph/s
Focal spot min	1 x 0.5 µm^2
Focal spot range	1 – 50 µm

Frontier Microfocusing MX

AMX

Energy range1	5 – 18 keV
Wavelength range	0.7 – 2.5 Å
Flux at focus	~2×10^{13} ph/s
Focal spot min	4 × 3 µm^2
Focal spot range	4 – 100 µm

Highly Automated MX

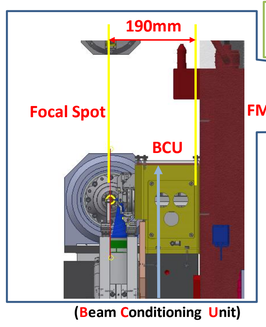


Sector: 17-ID @ NSLS-II
Source: Two canted IVU-21 Undulators

FMX & AMX's **specific & new features**
- Micro focus beams
- High energy
- Automation
- High flux
- Next Generation Pixel Array Detectors

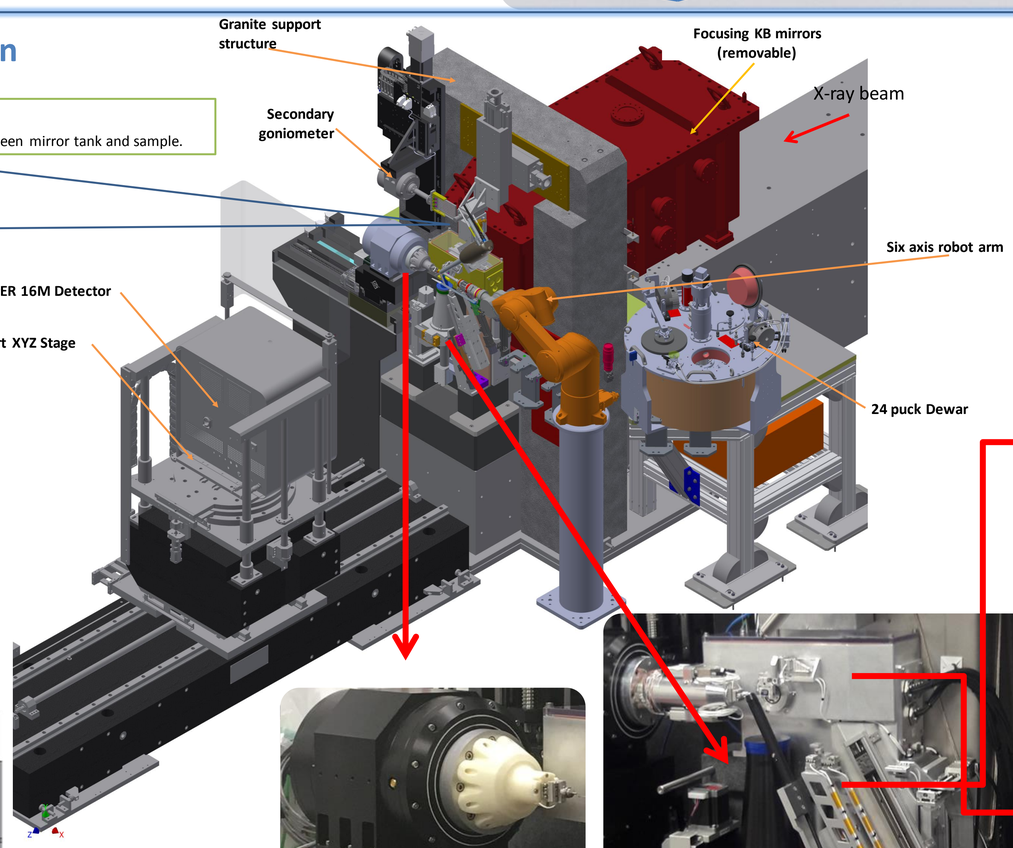
research instruments

FMX Experimental Station

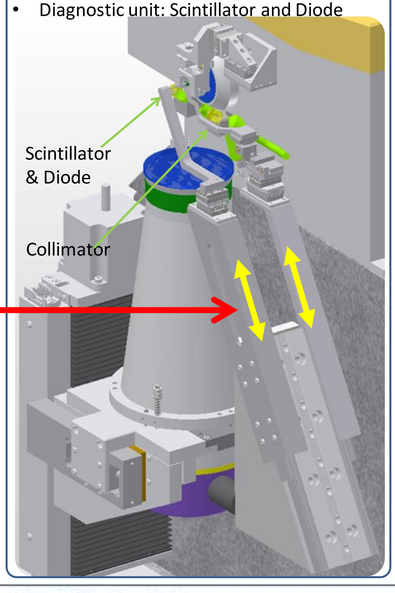


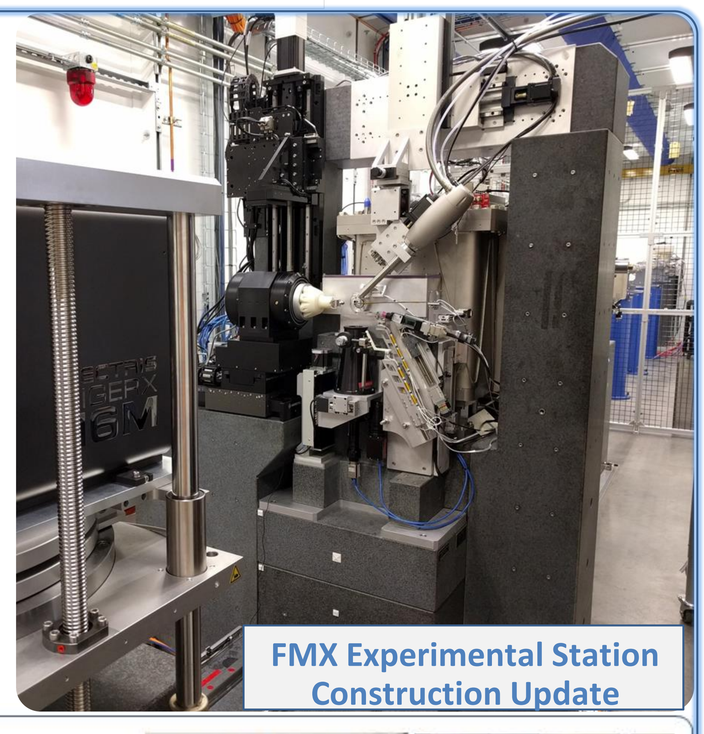
(Beam Conditioning Unit)

Challenge:
Just 190mm between mirror tank and sample.



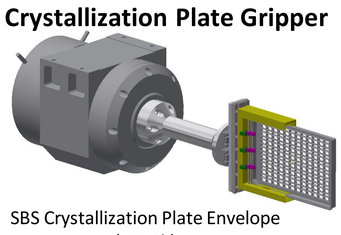
Beam shaping
(similar for both FMX and AMX End Stations)
- Collimator on flexural platform to shield x-rays
- Diagnostic unit: Scintillator and Diode



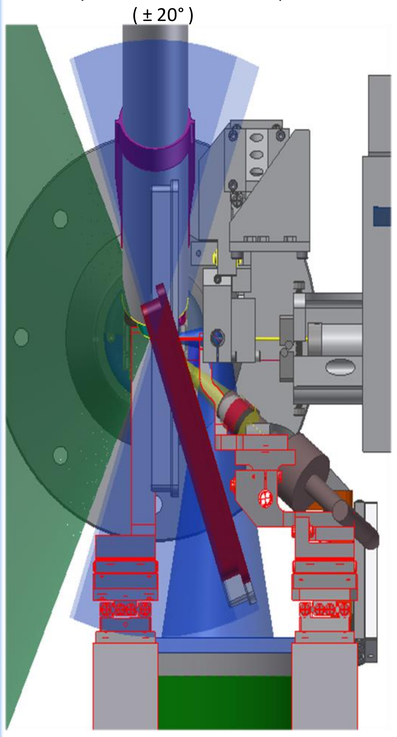


FMX Experimental Station Construction Update

Crystallization Plate Gripper



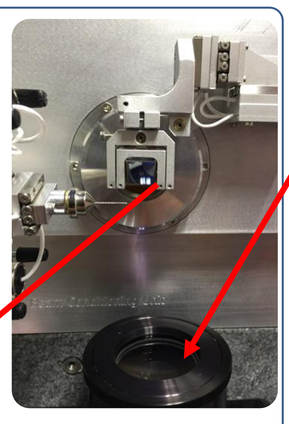
SBS Crystallization Plate Envelope
(± 20°)



Main Goniometer Arm
SOC target: 100nm on Nelson Air bearing

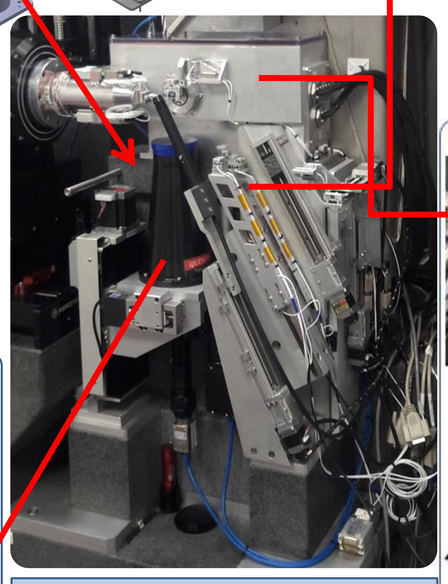
Sample visualization

FMX/AMX end stations will provide
- Diffraction-based crystal alignment and mapping
- On-axis microscope
- UV-excited fluorescence imaging



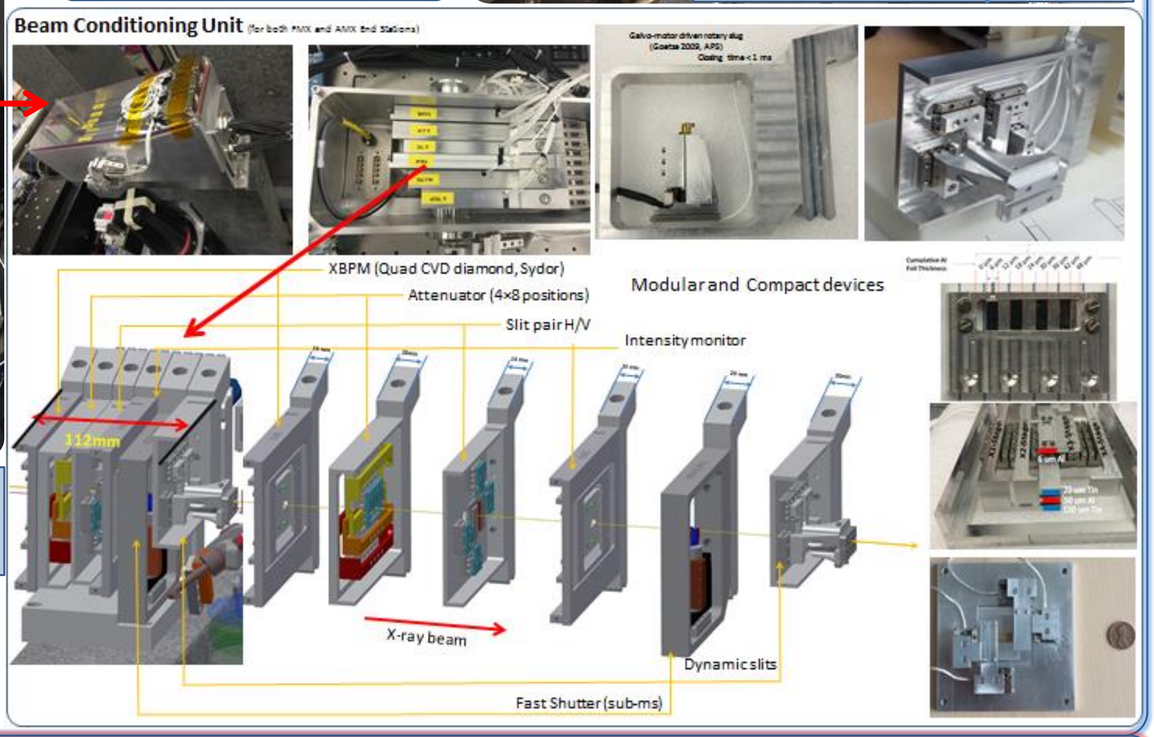
Flexural deflection mirror stage

(Custom Questar QM 100 telescope)
Gofron, K. J. & Duke, N. E. C. "Using X-ray excited UV fluorescence for biological crystal location"
Nucl. Instr. and Meth. A, (2011) **649** 216-218

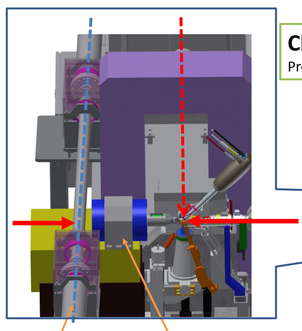


FMX Core Module
(similar construction for AMX)

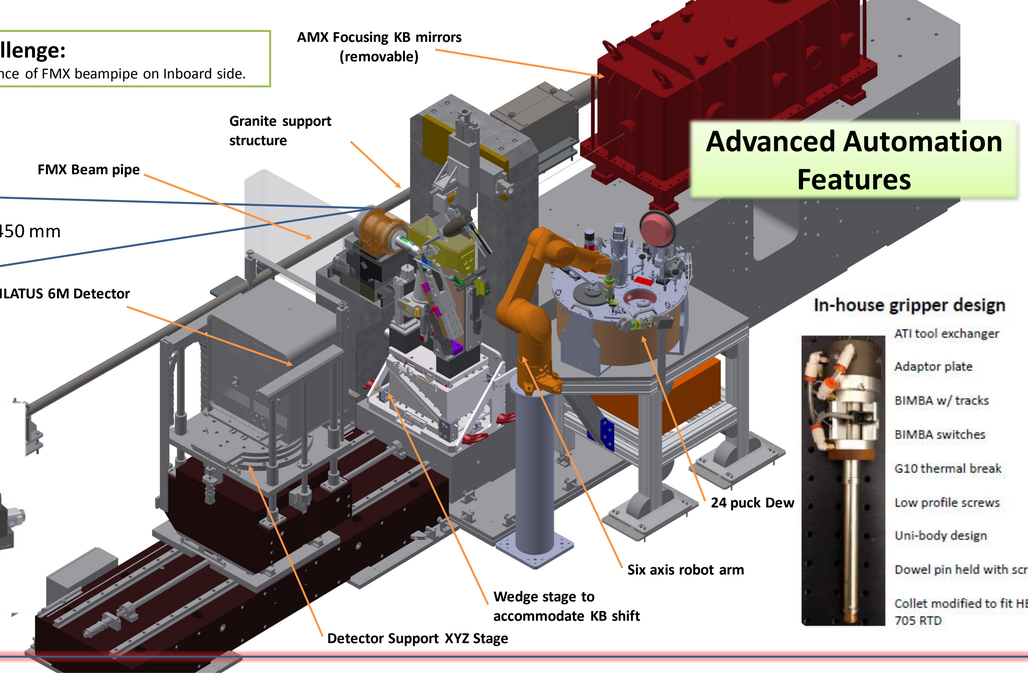
Beam Conditioning Unit (for both FMX and AMX End Stations)



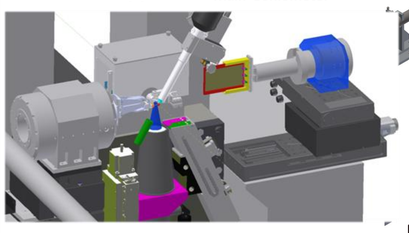
AMX Experimental Station



Challenge:
Presence of FMX beampipe on Inboard side.



Advanced Automation Features



AMX secondary goniometer (optional)

In-house gripper design

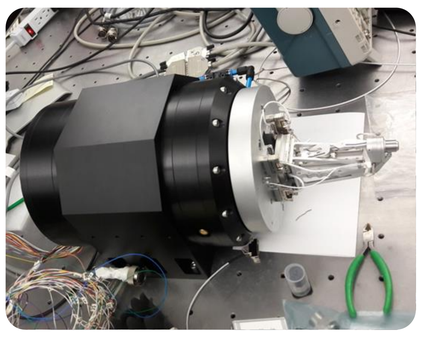
ATI tool exchanger
Adaptor plate
BIMBA w/ tracks
BIMBA switches
G10 thermal break
Low profile screws
Uni-body design
Dowel pin held with screws
Collet modified to fit HEL-705 RTD

Multi-axis goniometry : SmarGon by SmarAct

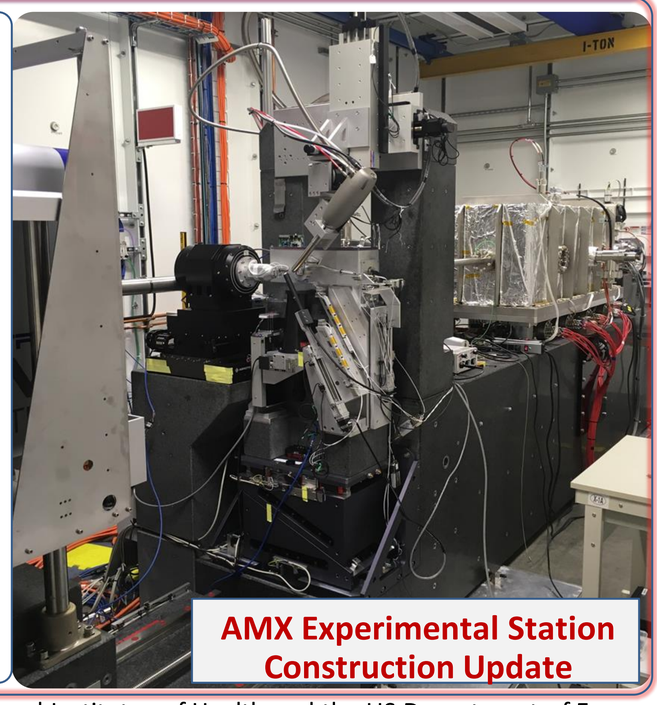
Formerly known as PRIGo:
Parallel Robotics Inspired Goniometer

Plans for implementation:
- AMX: SmarGon on main axis
- FMX: SmarGon on secondary goniometer

➢ SLS technology licensed to SmarAct



- SLS PRIGo: Omega SOC < 1 µm
- ➢ On SP150 Nelson Air Bearing.



AMX Experimental Station Construction Update

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