

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

Dileep K. Bhogadi, Martin R. Fuchs, Jean Jakoncic, Babak Andi, Stu Myers, James Magill, Mary Carlucci-Dayton, Lonny E. Berman, Dieter K. Schneider, Bob M. Sweet and Sean McSweeney

National Synchrotron Light Source II, Brookhaven National Laboratory, Upton NY, 11973, USA
 dbhogadi@bnl.gov



MECHANICAL ENGINEERING DESIGN OF SYNCHROTRON RADIATION EQUIPMENT AND INSTRUMENTATION



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

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

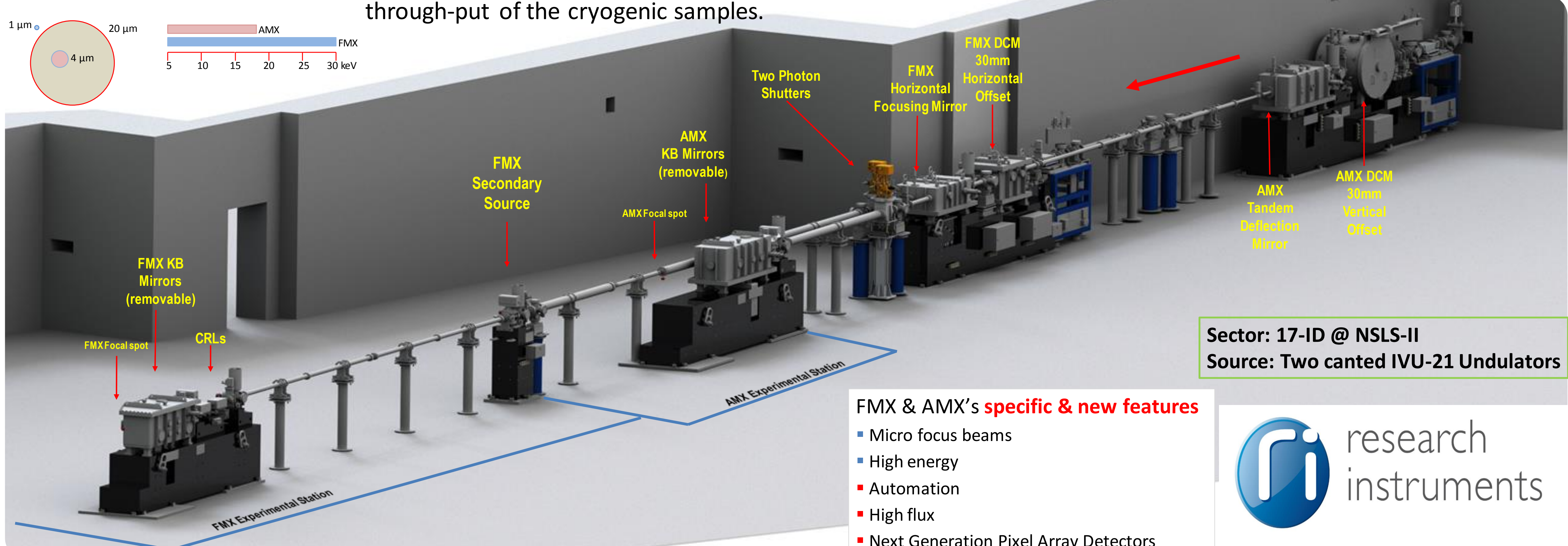
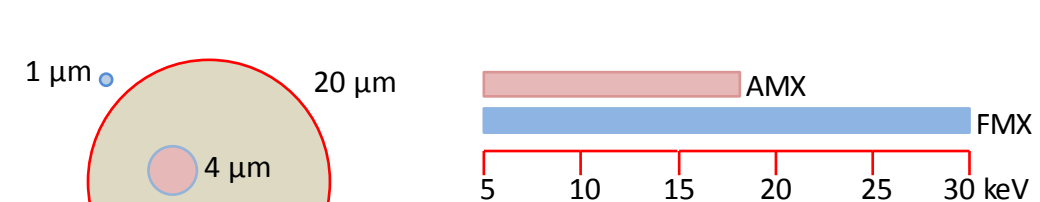
FMX

Frontier Microfocusing MX

| | |
|------------------|------------------------------|
| Energy range1 | 5 – 18 keV |
| Wavelength range | 0.7 – 2.5 Å |
| Flux at focus | $\sim 2 \times 10^{13}$ ph/s |
| Focal spot min | 4 x 3 μm^2 |
| Focal spot range | 4 – 100 μm |

AMX

Highly Automated MX

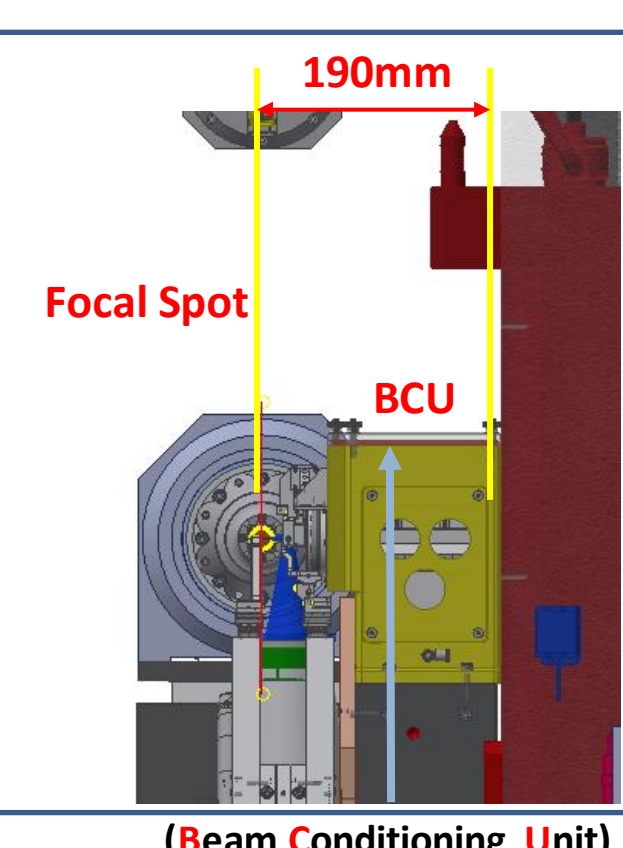


Sector: 17-ID @ NSLS-II
 Source: Two canted IVU-21 Undulators

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

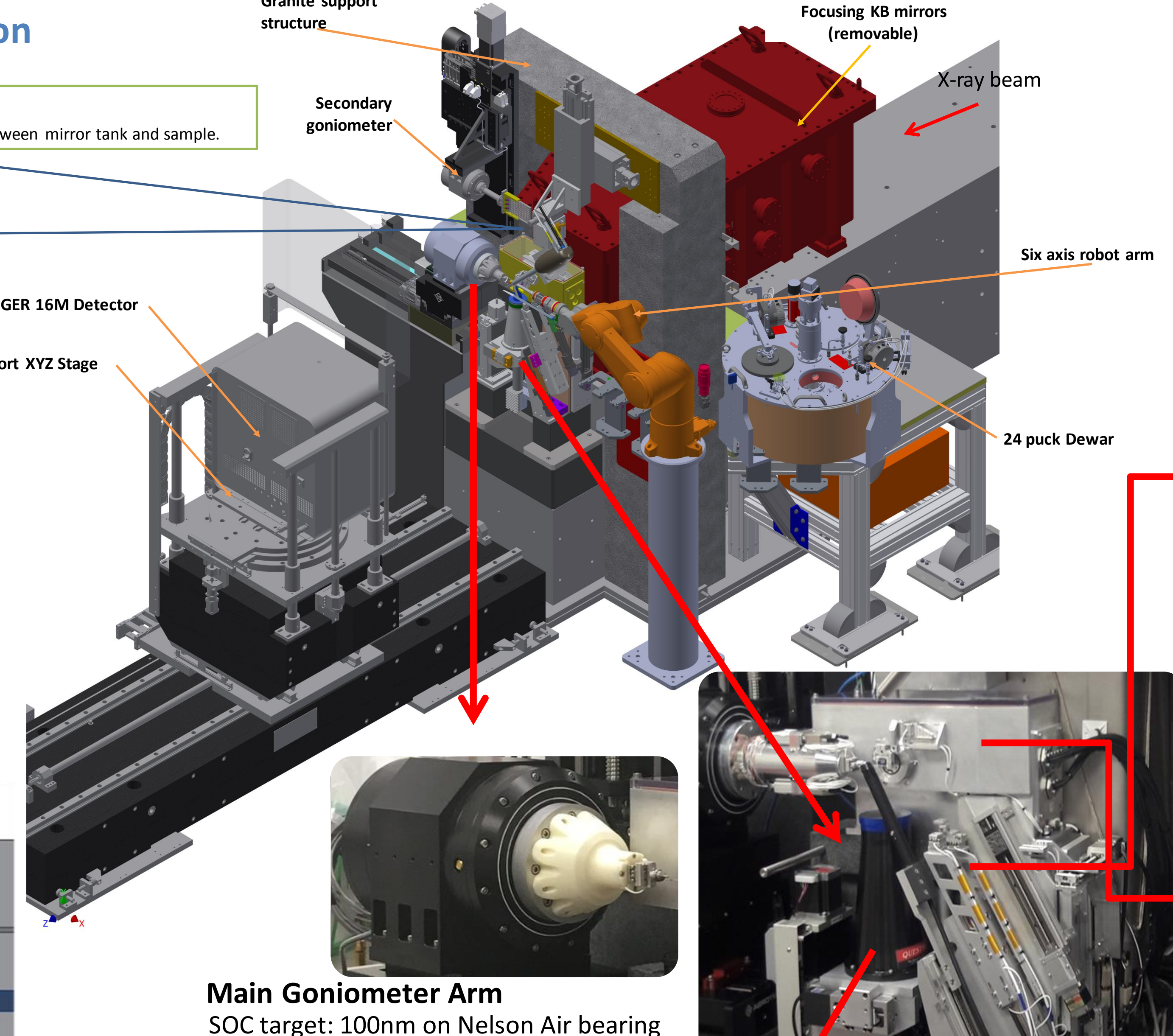
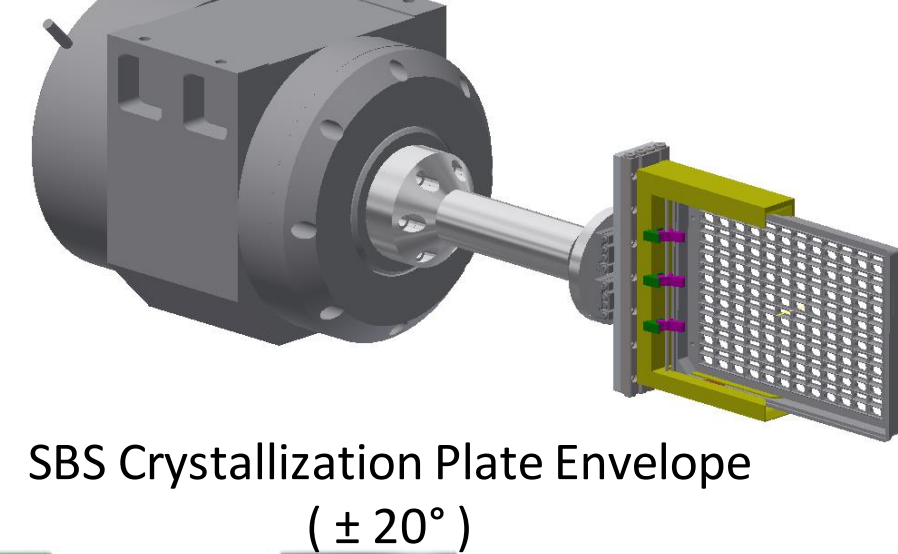


FMX Experimental Station



Challenge:
 Just 190mm between mirror tank and sample.

Crystallization Plate Gripper



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

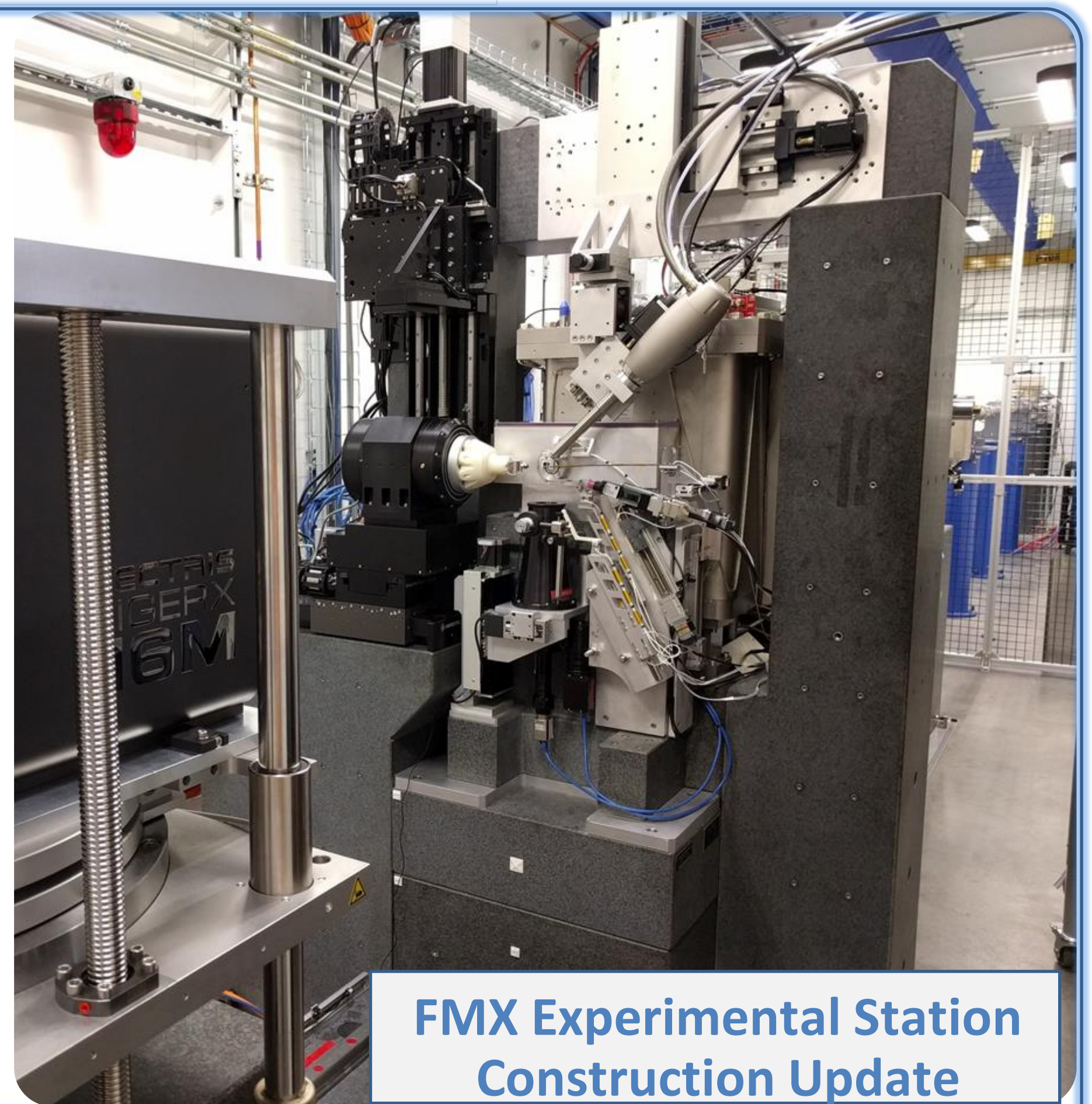
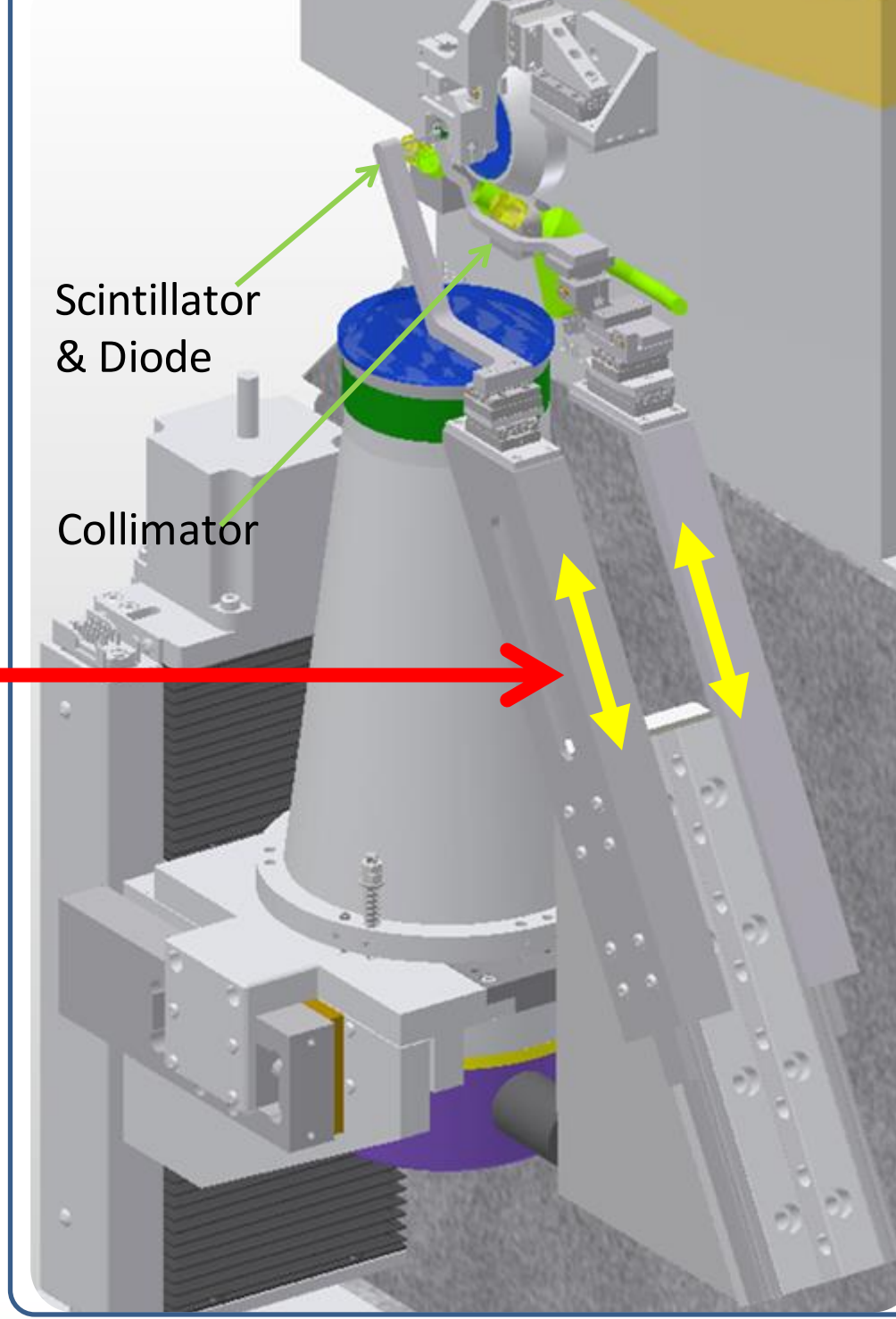
Sample visualization

- 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

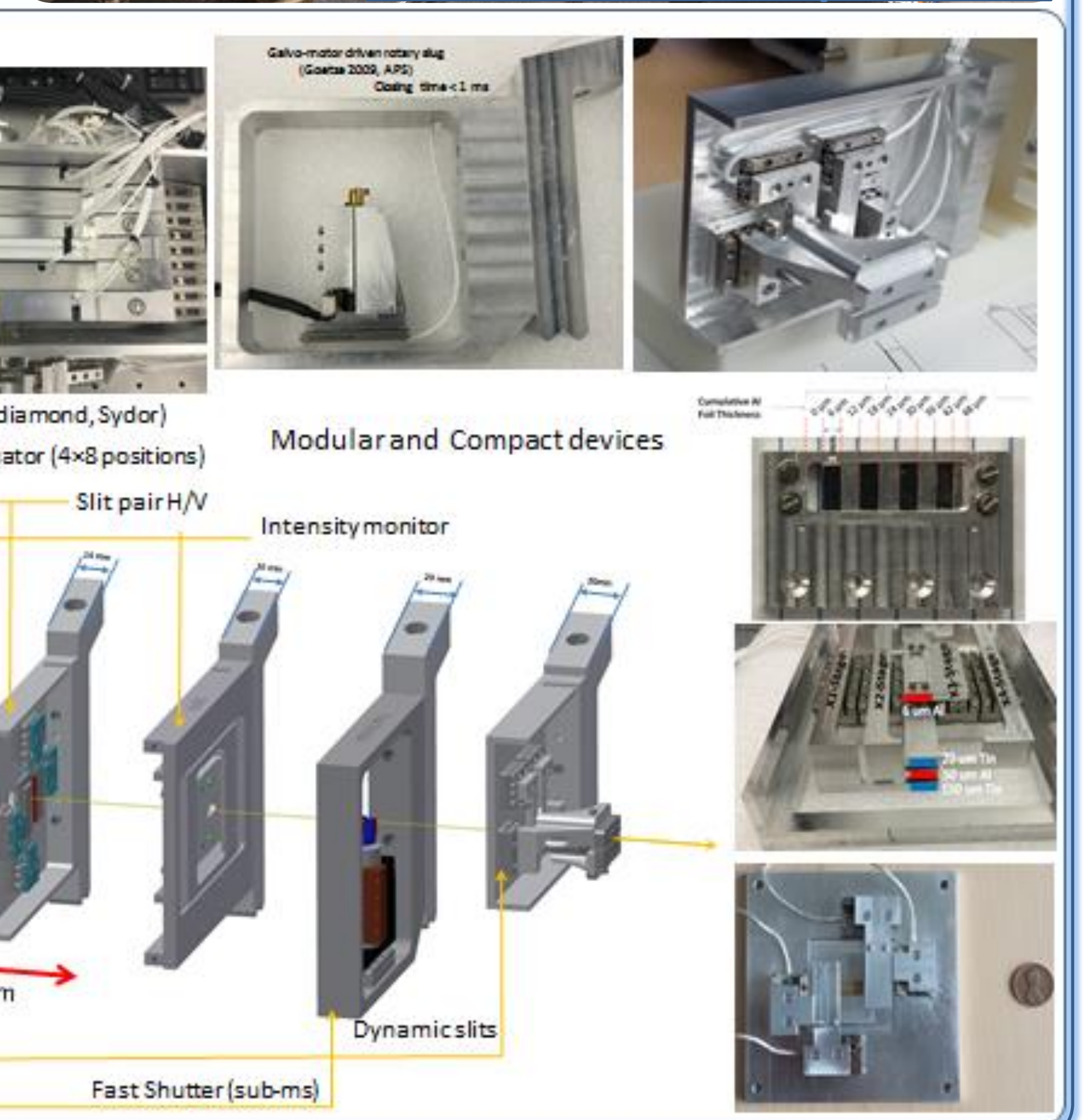
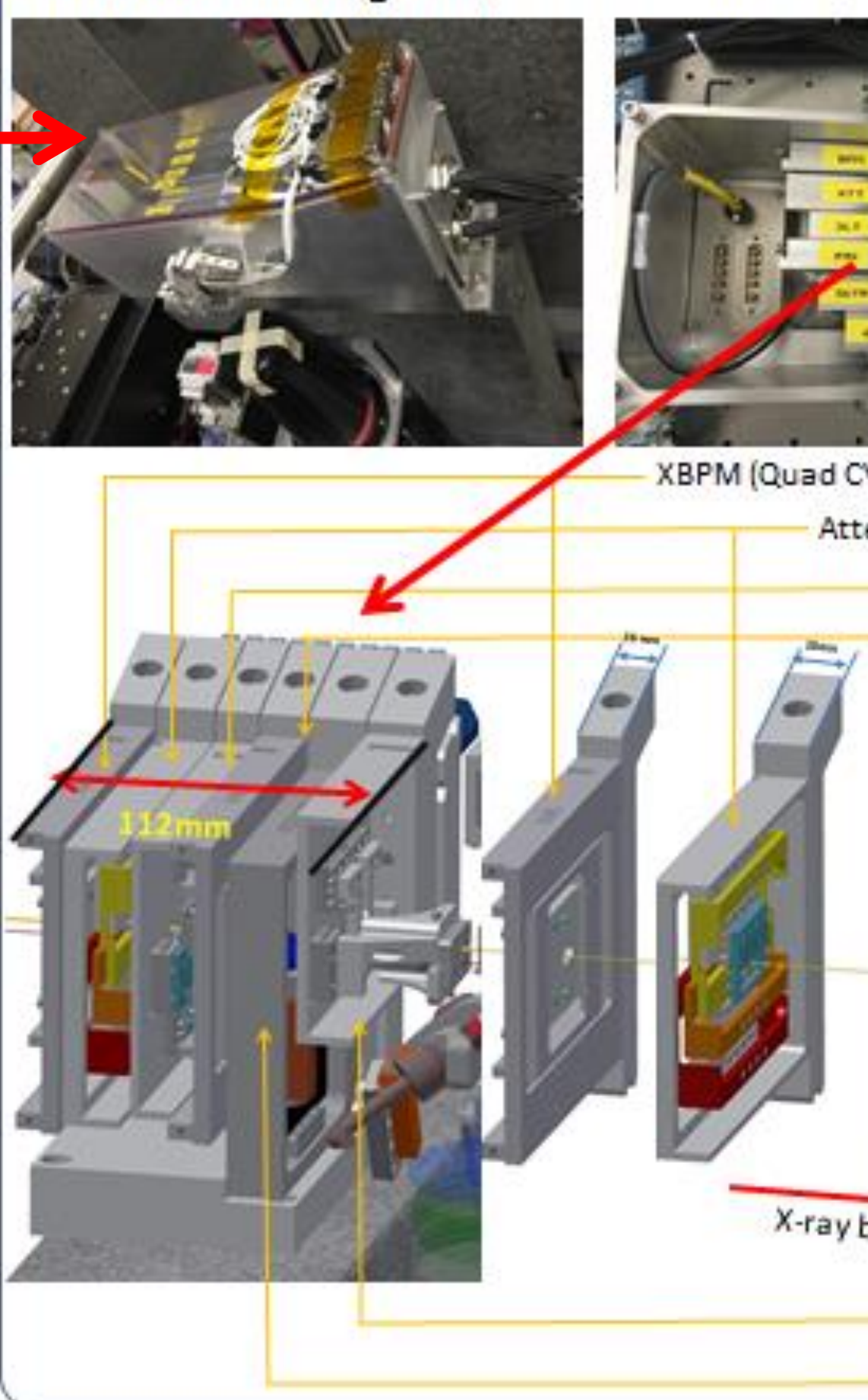
Beam shaping

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

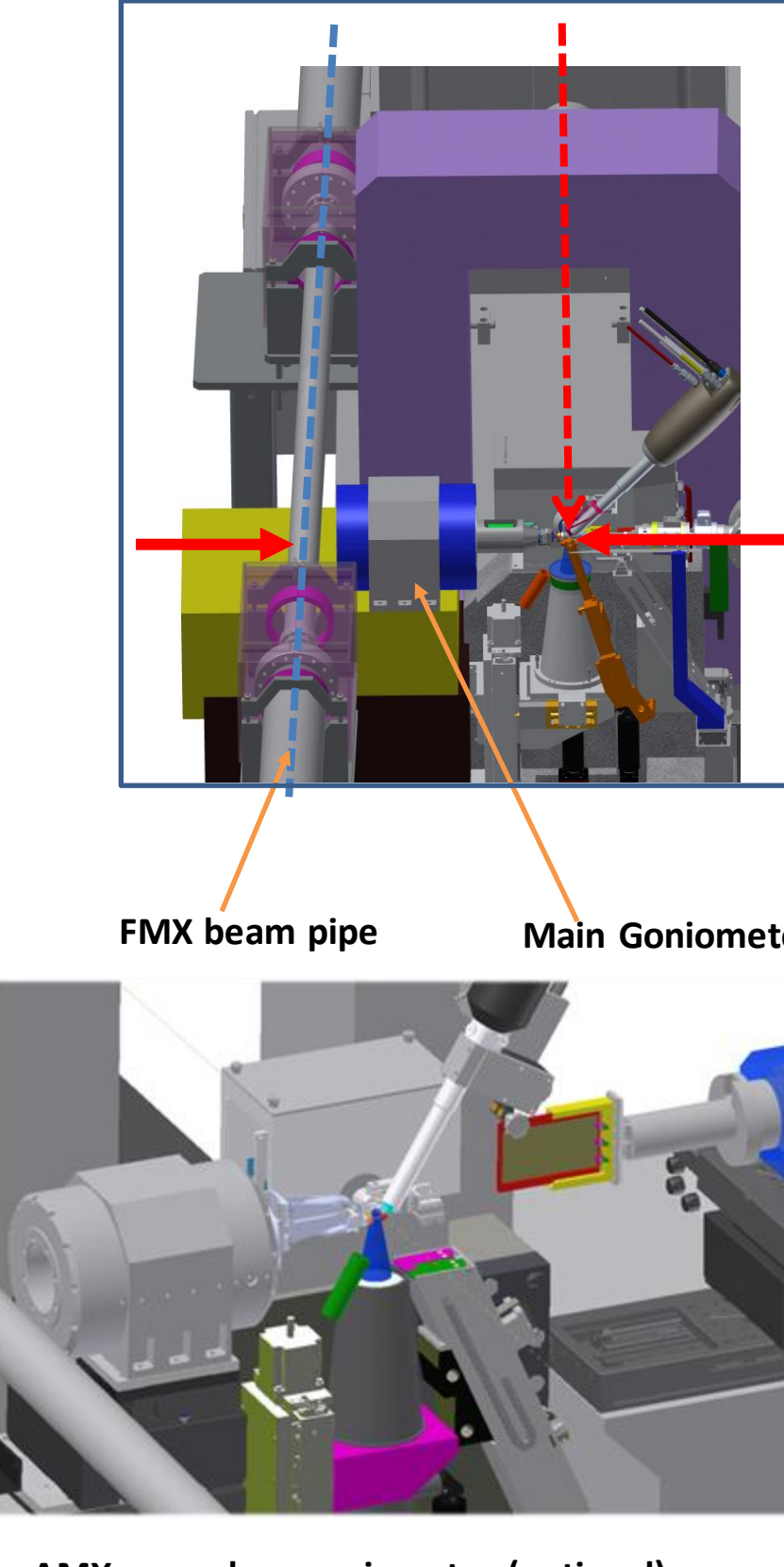


FMX Experimental Station Construction Update

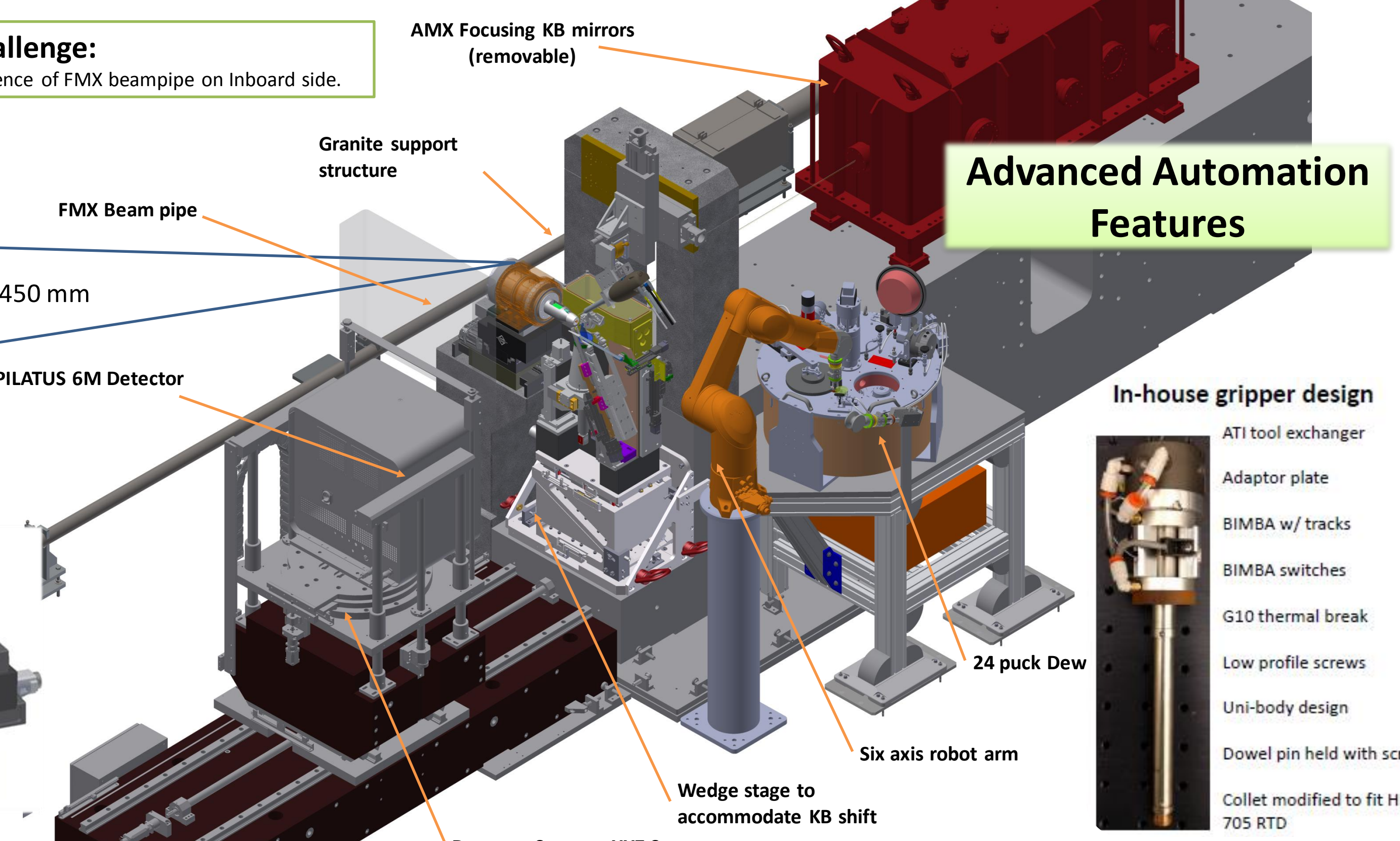
Beam Conditioning Unit



AMX Experimental Station



Challenge:
 Presence of FMX beam pipe on Inboard side.

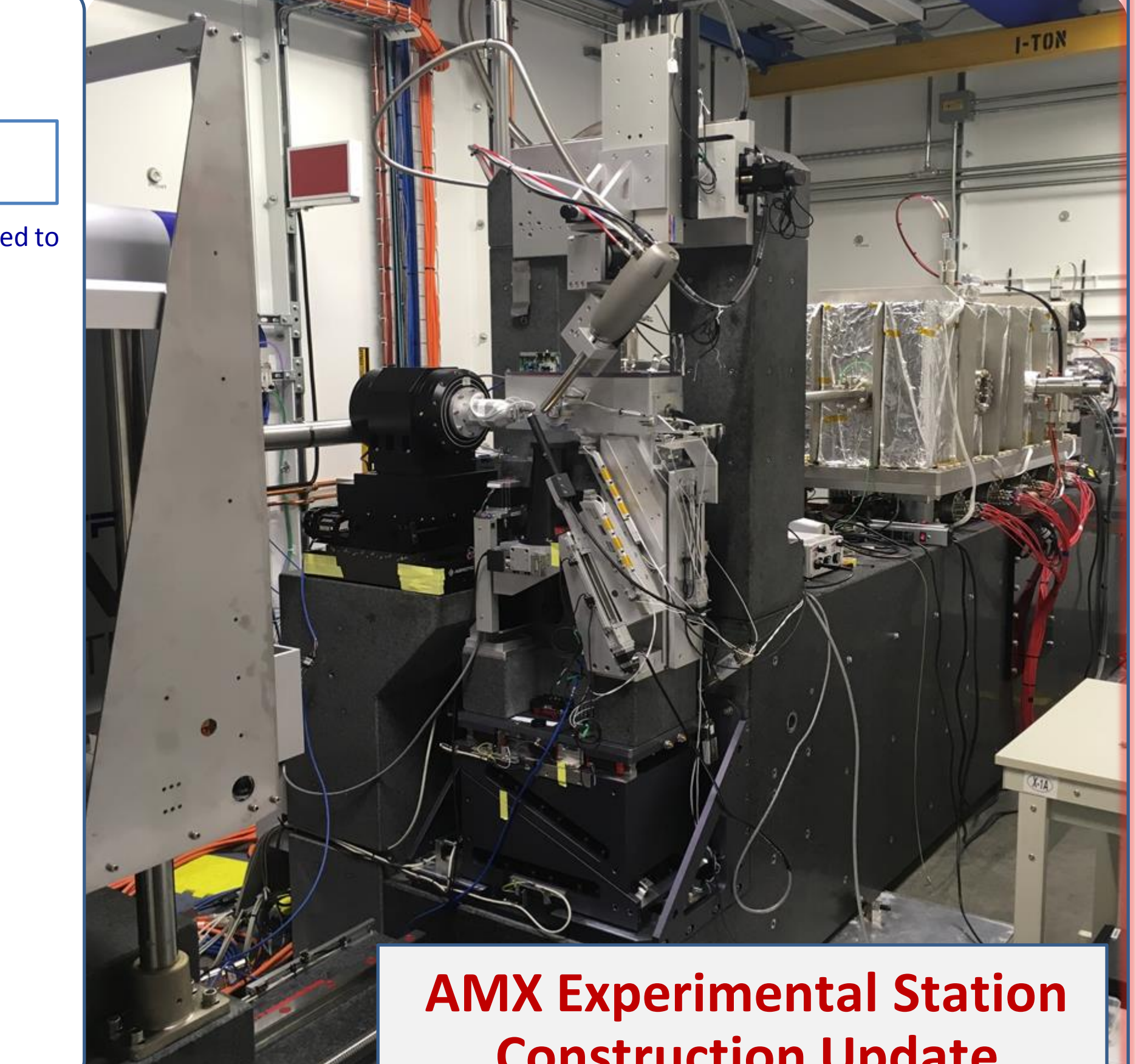


Advanced Automation Features

- 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