OAK RIDGE National Laboratory | SECOND TARGET STATION

QIKR Instrument Overview

John F. Ankner
QIKR Instrument Scientist

QIKR Shielding Preliminary Design Review
March 3, 2025

Outline

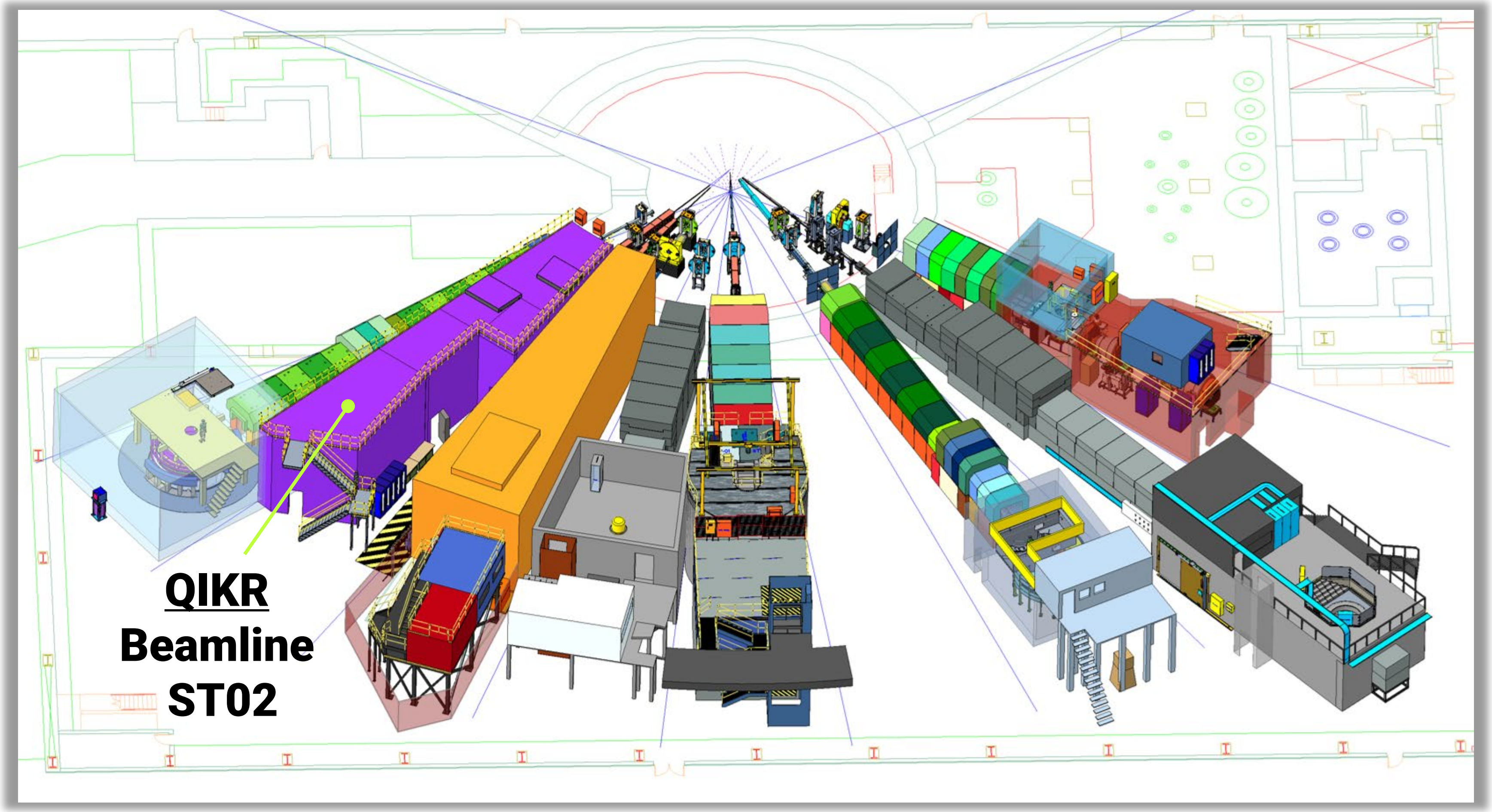
- QIKR, Briefly
- Unwanted Neutrons
  - Lost in monolith and bunker
  - Lost in instrument cave
- Summary

Outline

- **QIKR, Briefly**
- Unwanted Neutrons
  - Lost in monolith and bunker
  - Lost in instrument cave
- Summary

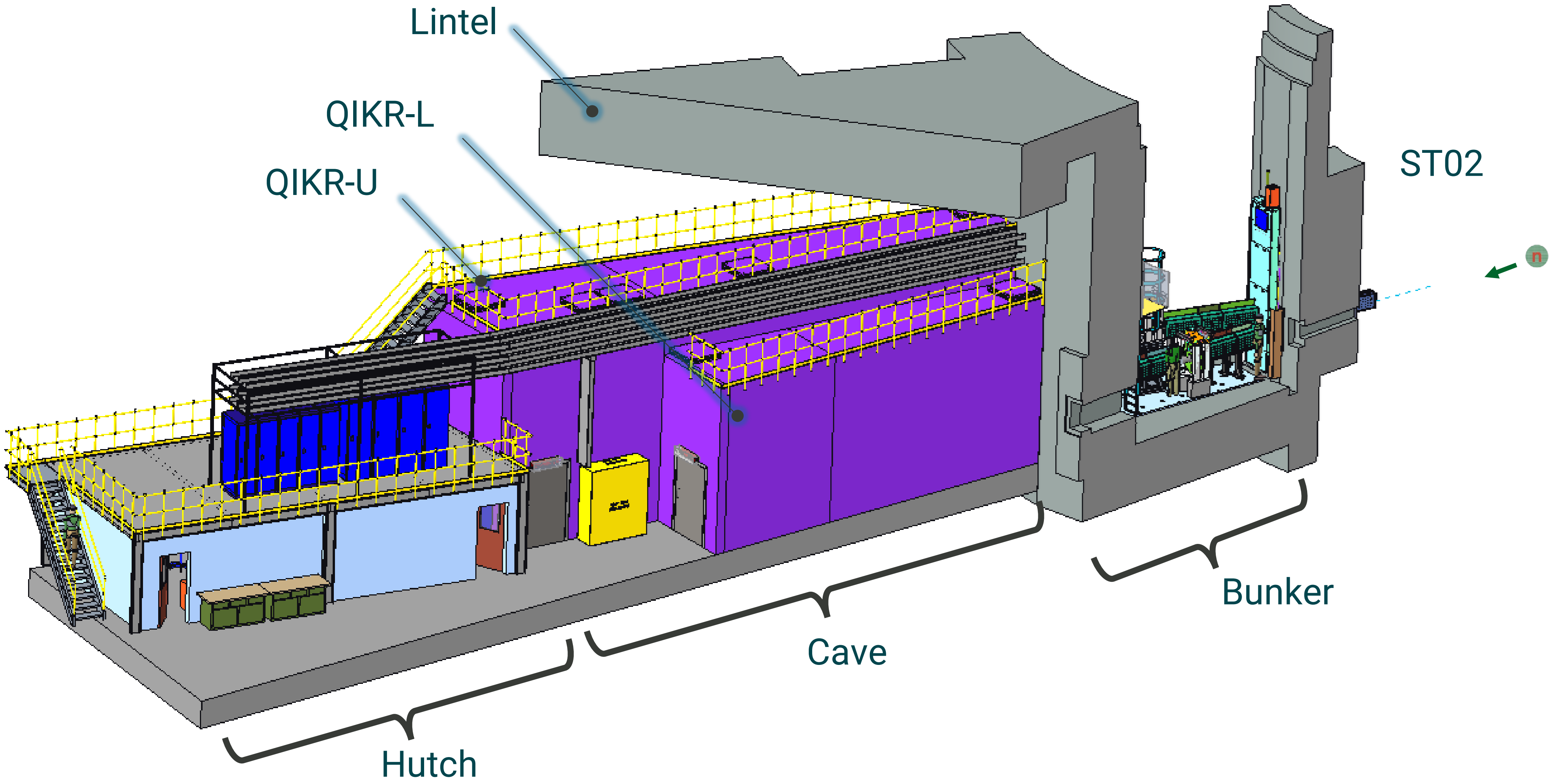
Location of QIKR

QIKR will sit at port ST02 and view the cylinder moderator

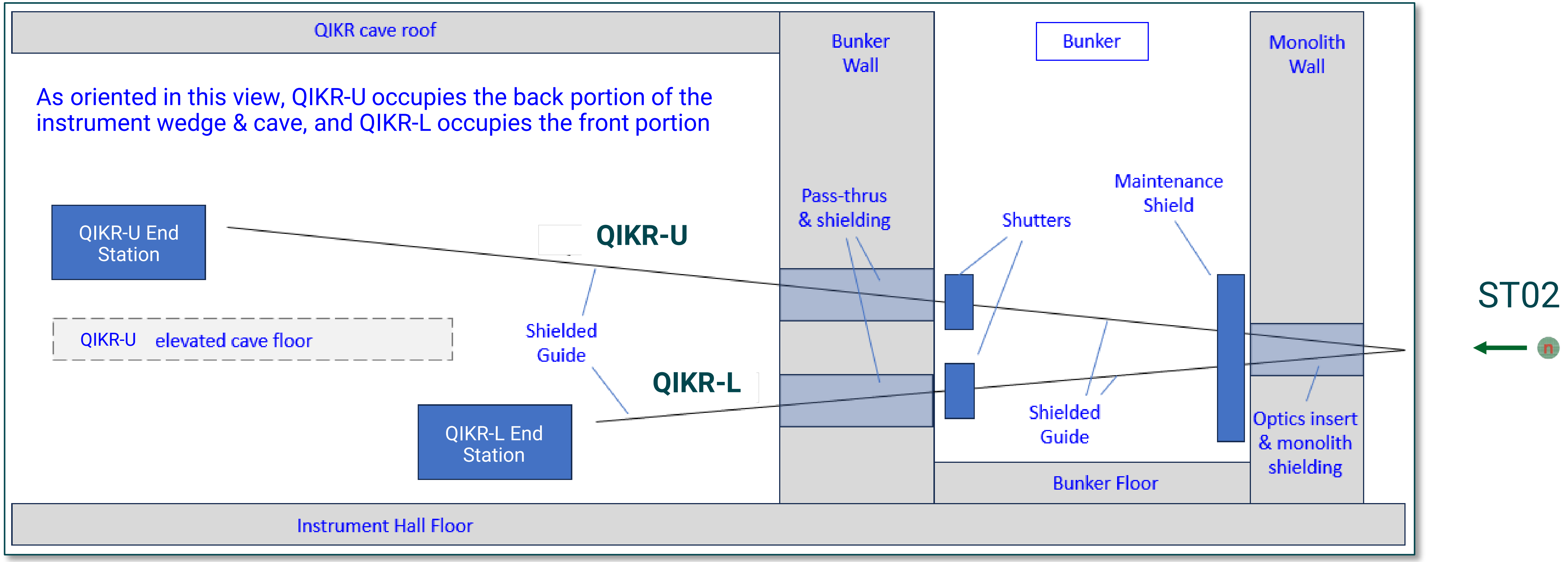


STS Beamlines in the South Instrument Hall

QIKR Instrument Sections



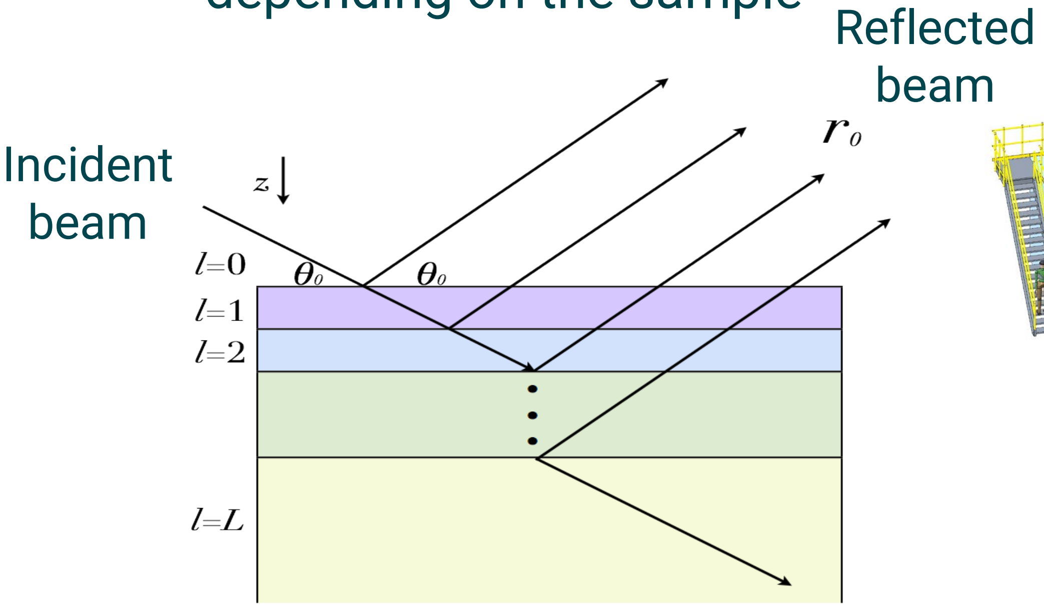
QIKR features two independent beamlines (schematic)



- The maintenance shield does <u>not</u> perform a beam blocking function
- The End Stations consist of an Incident Table with Slits, a Sample Table, and a Detector Arm

QIKR will make time-resolved reflectometry routine

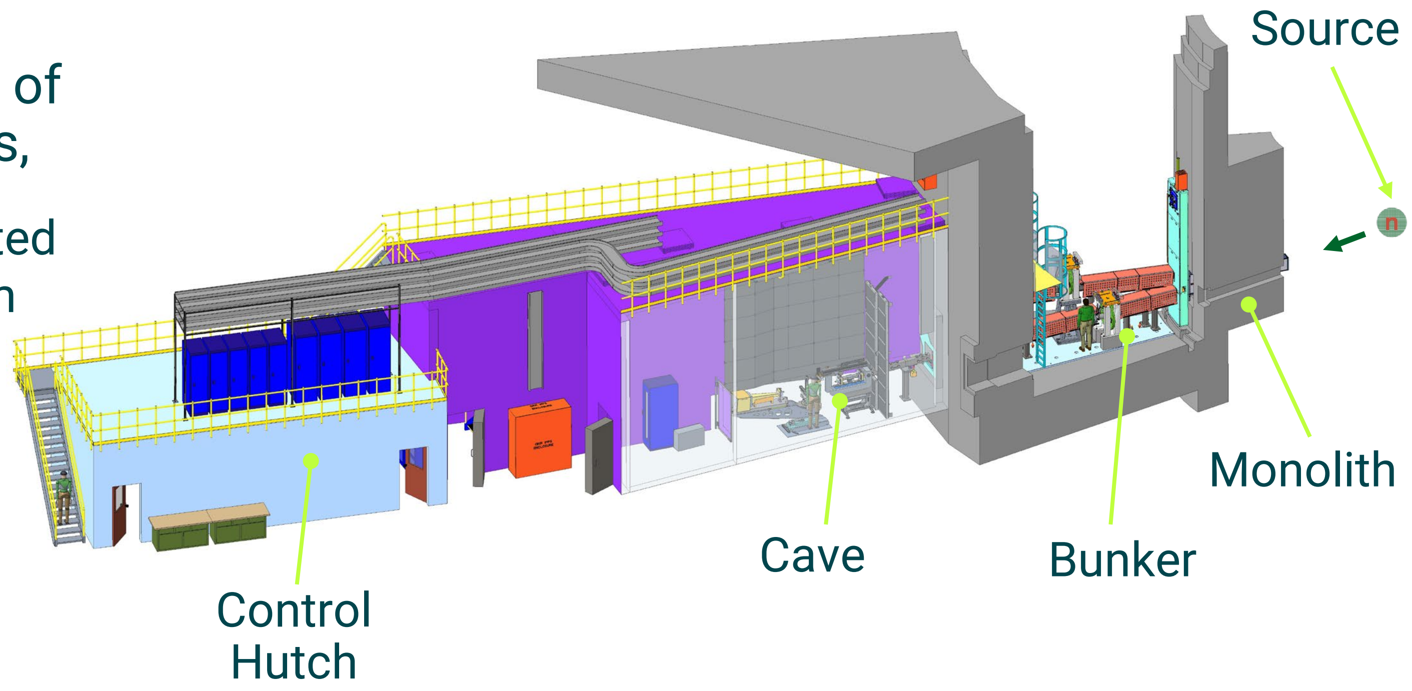
STS flux and wavelength bandwidth will enable routine single-setting measurement of specular reflectivity in seconds to minutes, depending on the sample



$$n_l = \sqrt{1 - \lambda^2 b_l / \pi V_l}$$

$$1/V_l = \frac{\rho_l N_A}{M_l}$$

[Density × Avogadro’s number / Molecular mass]



“Cinematic” data collection at one instrument setting and event-based data reduction will enable post-experiment tracking of structural evolution in time over a broad scientific landscape

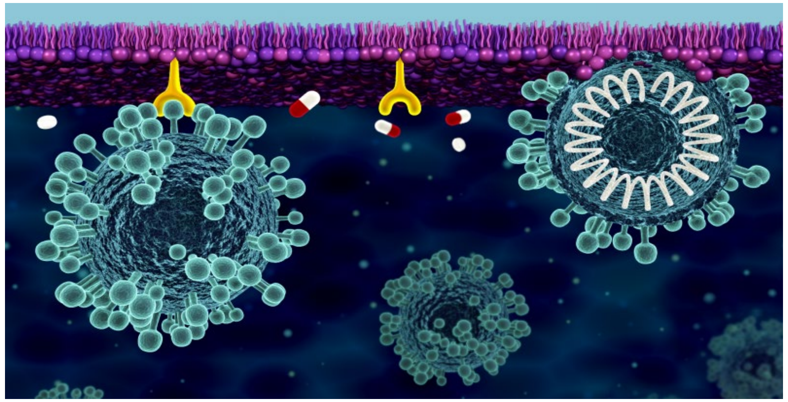
A sampling of scientific communities served by QIKR

Soft Matter

- Polymer diffusion
- Chemical transformation of reactive films
- Hydrogels
- Fouling
- Structure-properties of films under shear
- Synthetic membranes
- Responsive films
- Polymer brushes under shear
- Surface modification
- Reactions at oil/water interfaces

Energy Materials

- Solid-electrolyte interphase
- Organic photovoltaics
- Ionic liquids
- Corrosion
- Mesoporous films
- Conjugated polymer films
- Metal-harvesting polymers



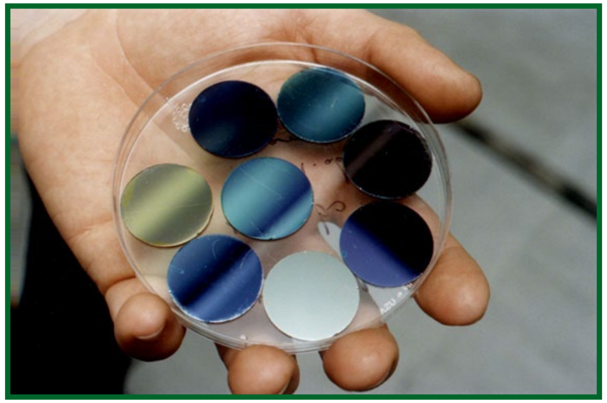
[Courtesy R. Ashkar]

Biomaterials

- Model membranes
- Lipid flip-flop
- Structure of transmembrane peptides
- Biocompatible coatings
- Surfactant and phospholipid monolayers
- Drug delivery
- Protein conformation to membranes
- Influence of synthetic nanoparticles on membrane structure

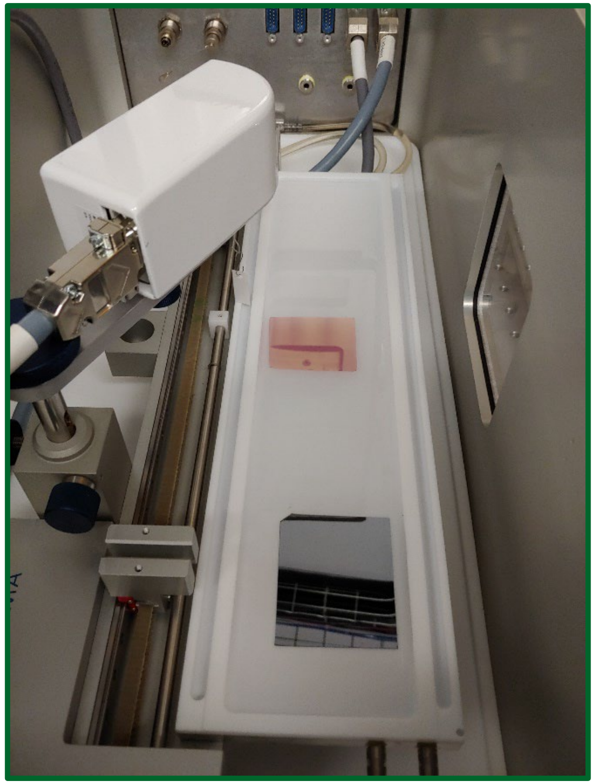
Nano-scale layers deposited on flat substrates

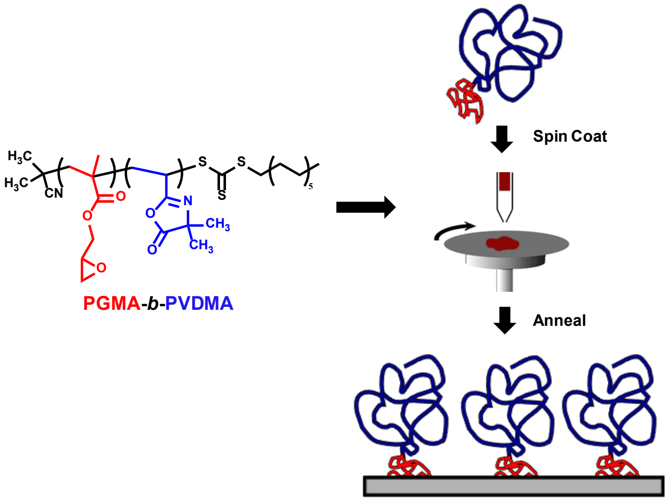
Layer-by-Layer Growth



Rheometry

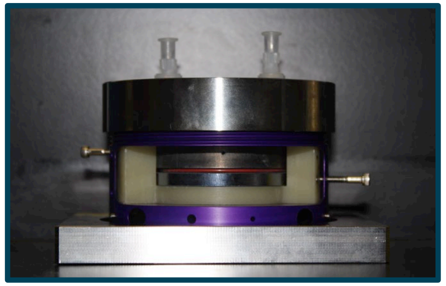
Langmuir Films

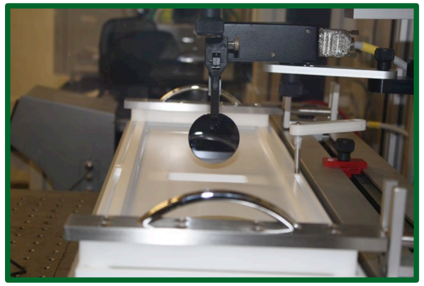




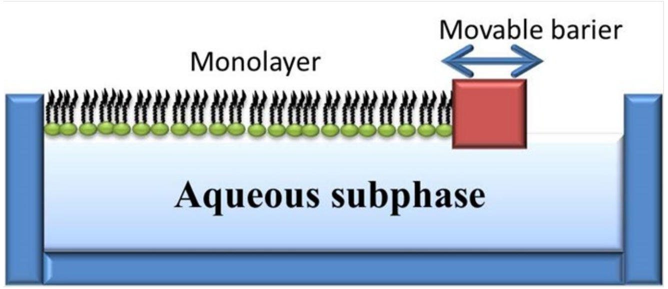
Spin Coating

Electrochemistry

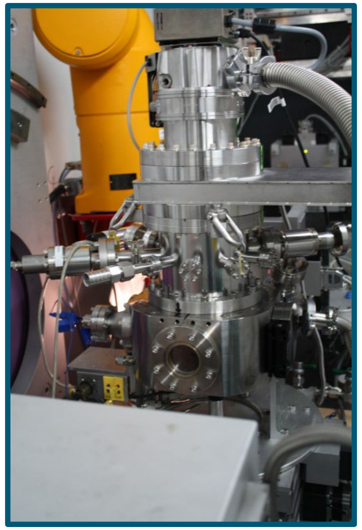


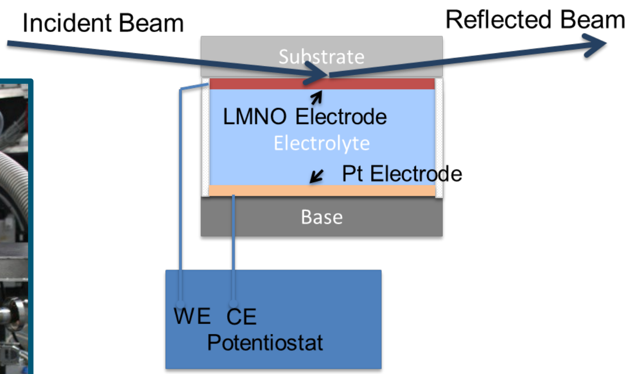


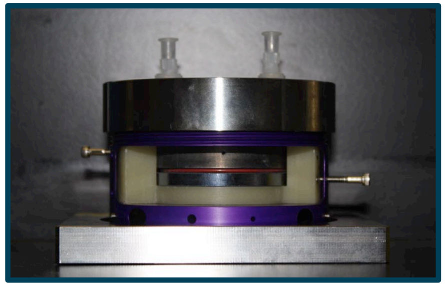
Langmuir-Blodgett deposition

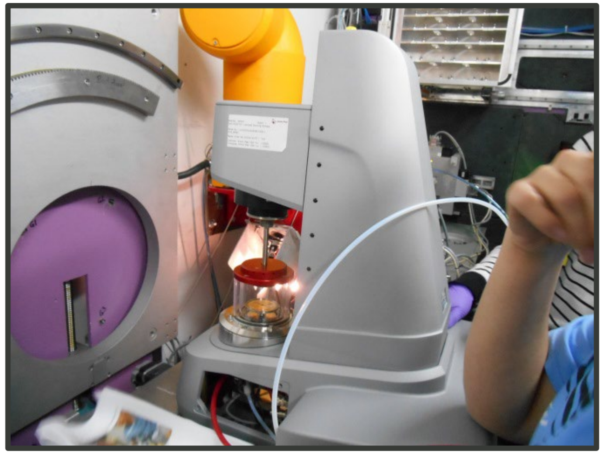


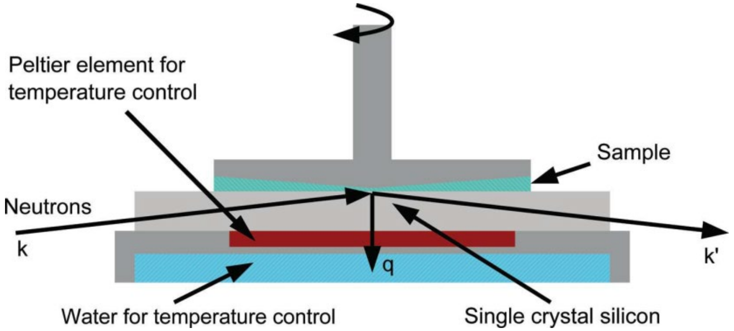
Diverse geometries







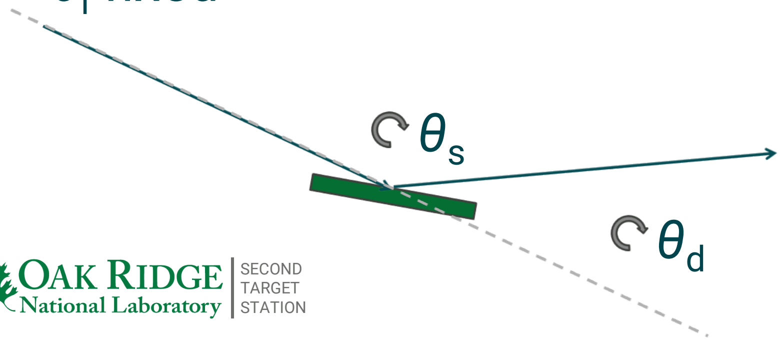


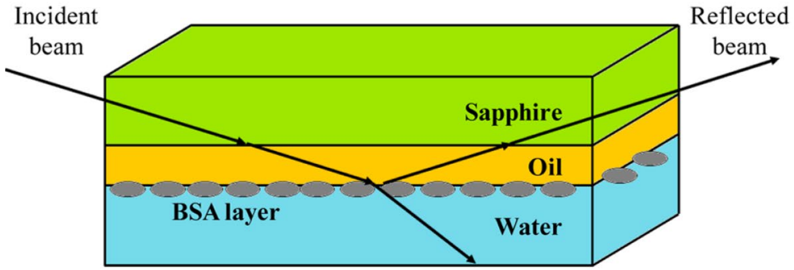


θ-2θ geometry

$\theta_d = 2\theta_s$

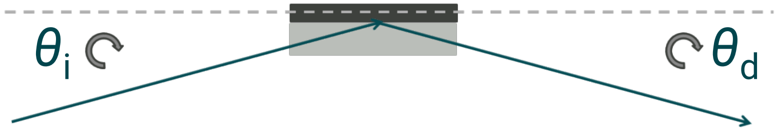
θ_i fixed





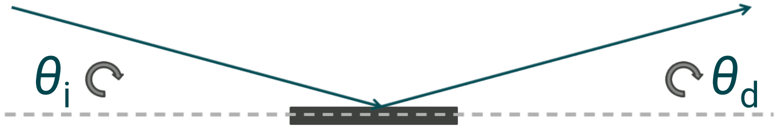
Two end stations

θ_s = 0, fixed



θ-θ geometry

$\theta_d = -\theta_i$



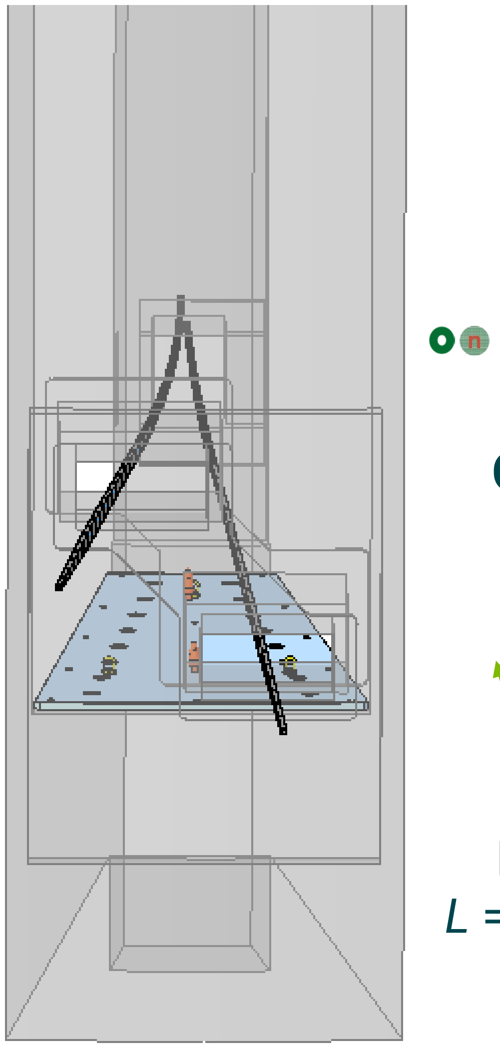
θ_s = 0, fixed

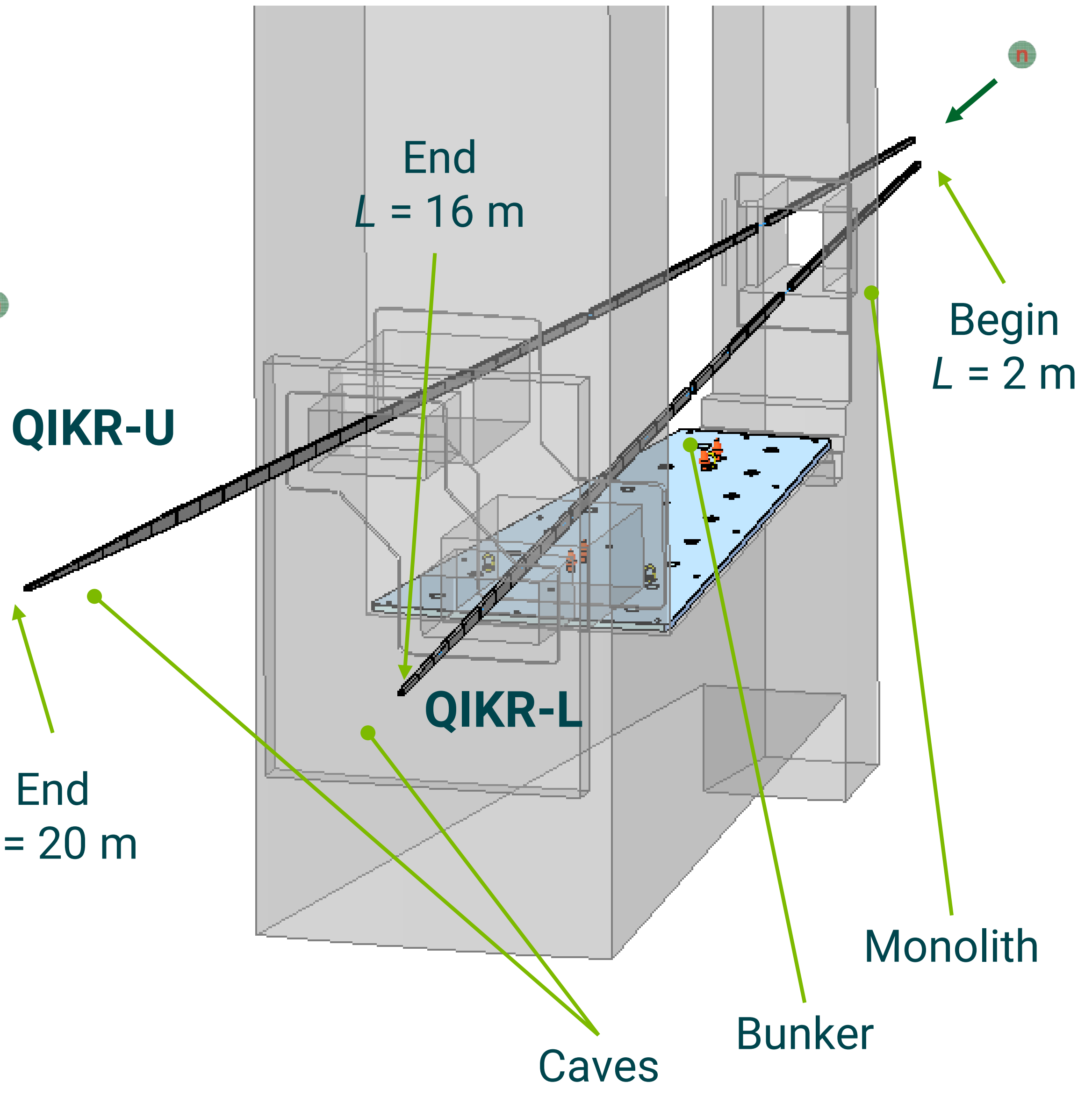
Oak Ridge National Laboratory

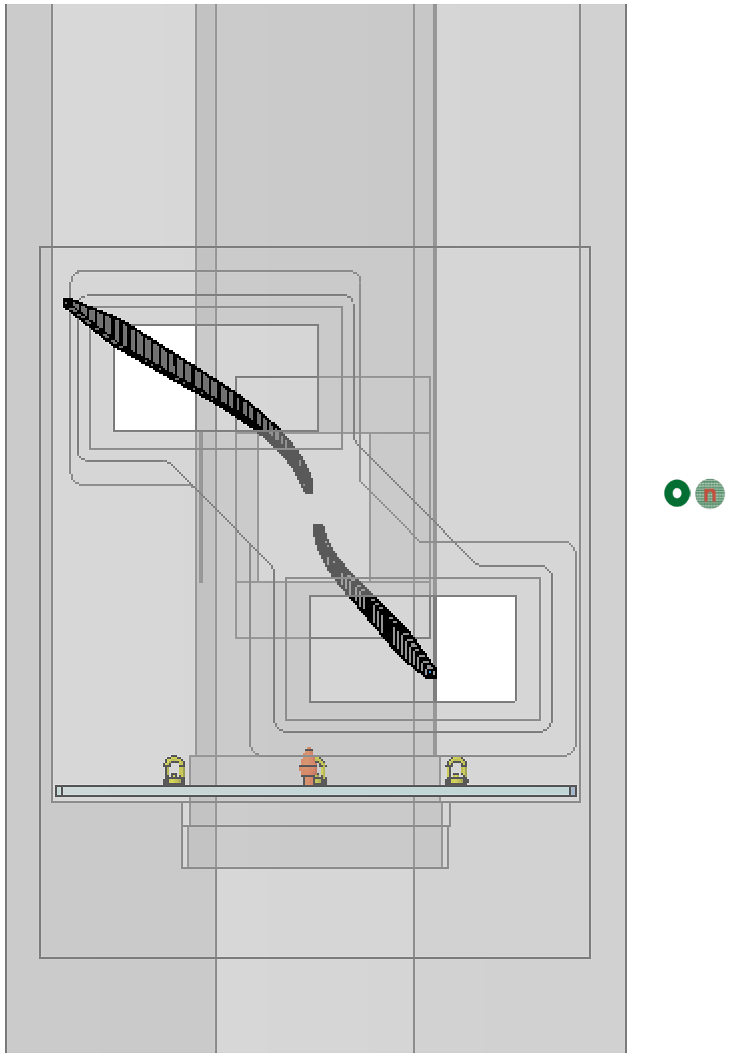
Outline

- QIKR, Briefly
- Unwanted Neutrons
  - **Lost in monolith and bunker**
  - Lost in instrument cave
- Summary

Guide views – looking upstream

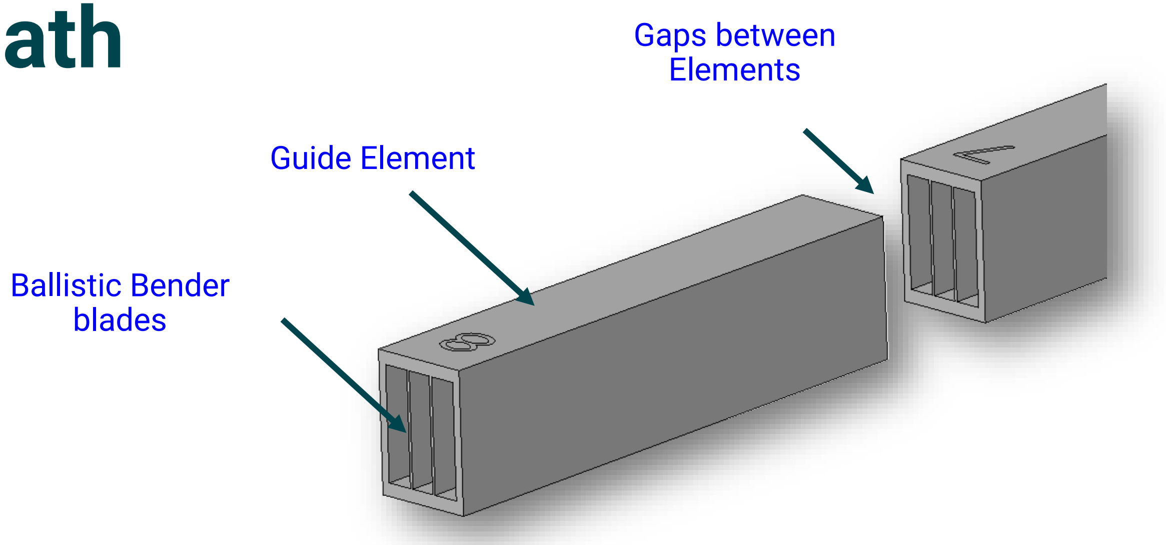


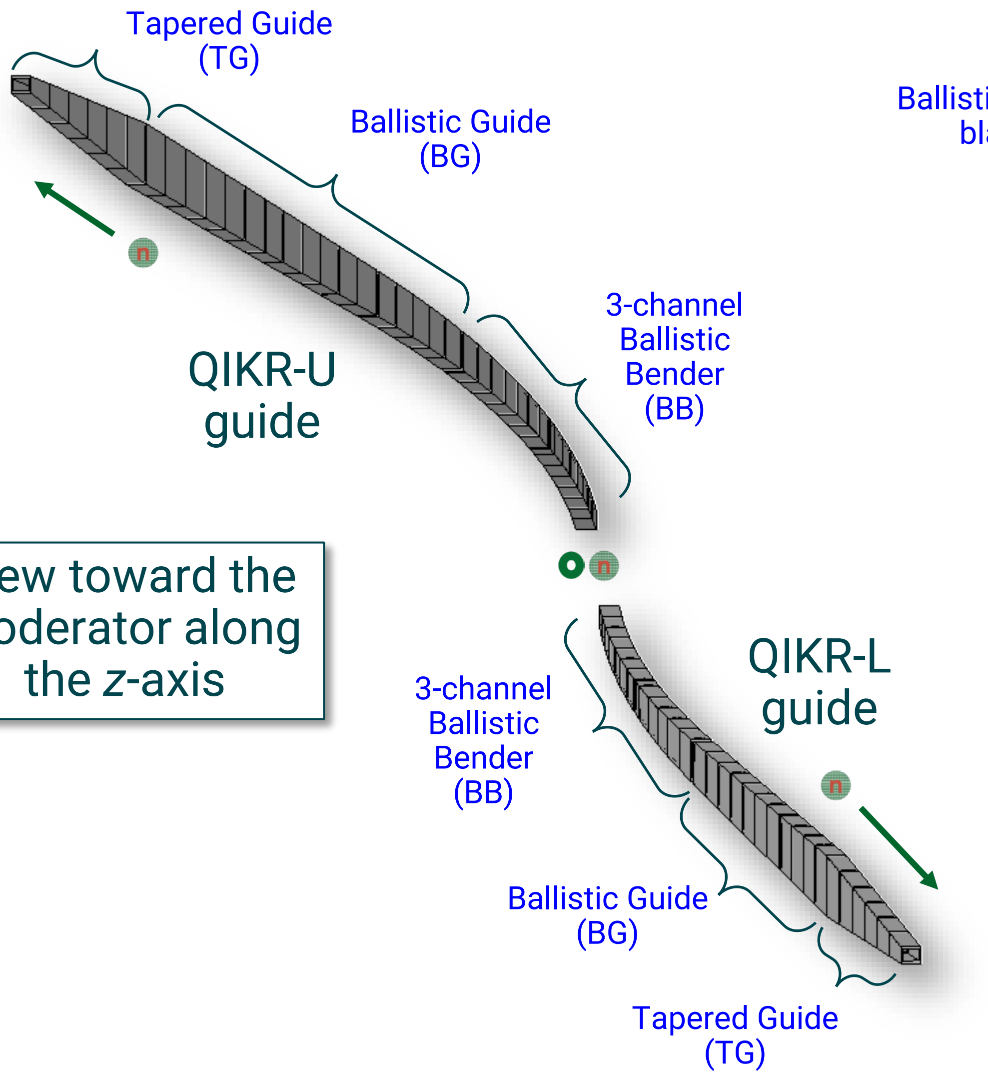




Guides taper, curve, and are angled up/down, left/right

QIKR Overview – Guide Path





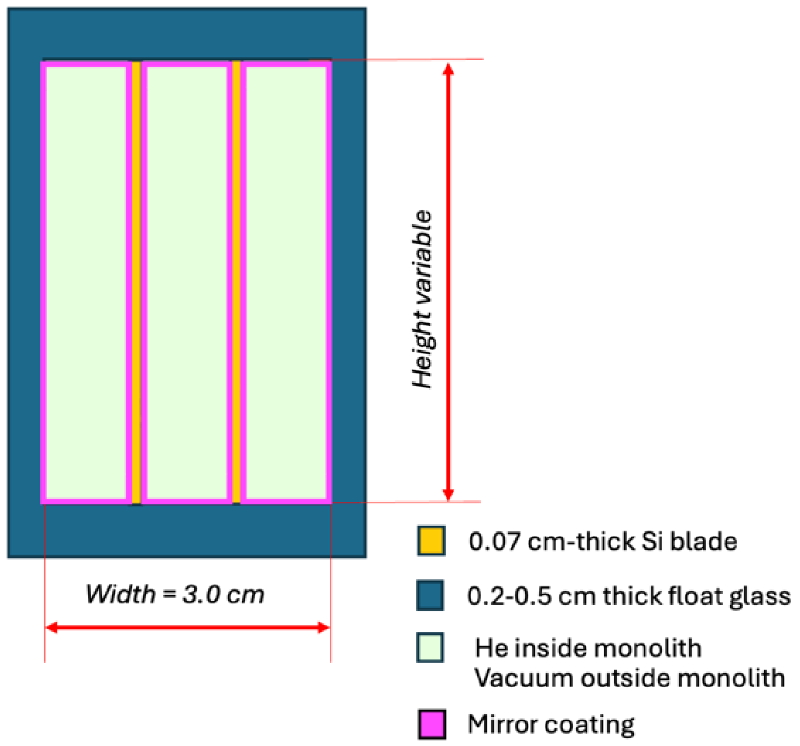
View toward the moderator along the *z*-axis

- Three sections in each guide path: Ballistic Bender (BB), Ballistic Guide (BG), and Tapered Guide (TG)
- Each guide Element is straight, even in the BB section
- In the BB section, each guide element is angled relative to its neighbor to approximate a 156-m radius circle
  - The initial 12 elements in each bender section are multichannel, the number of channels = 3
- The upper guide initially angles up by 2.5° and rotated by 0.7° toward ST01
- The lower guide angles down by 2.5° and rotated by 0.5° toward ST03

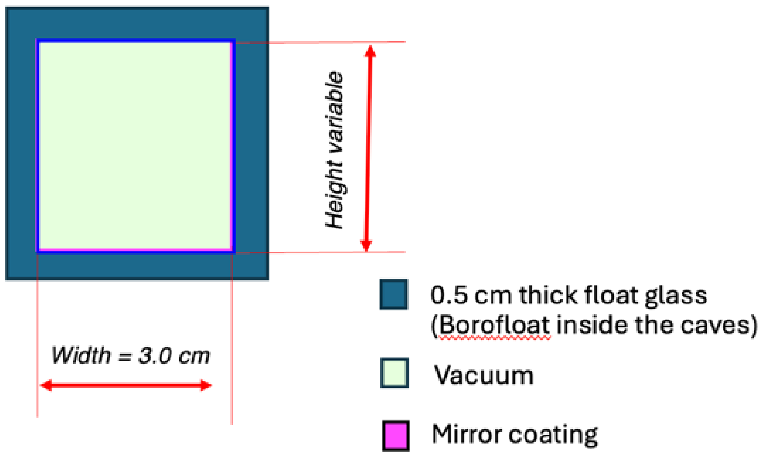
Guide representation in MCNP

Neutron guide transport calculated using a common STS source and dimensions and coordinates transferred from the engineering model (Creo->IGES) to both McStas and MCNP agreed within 15%

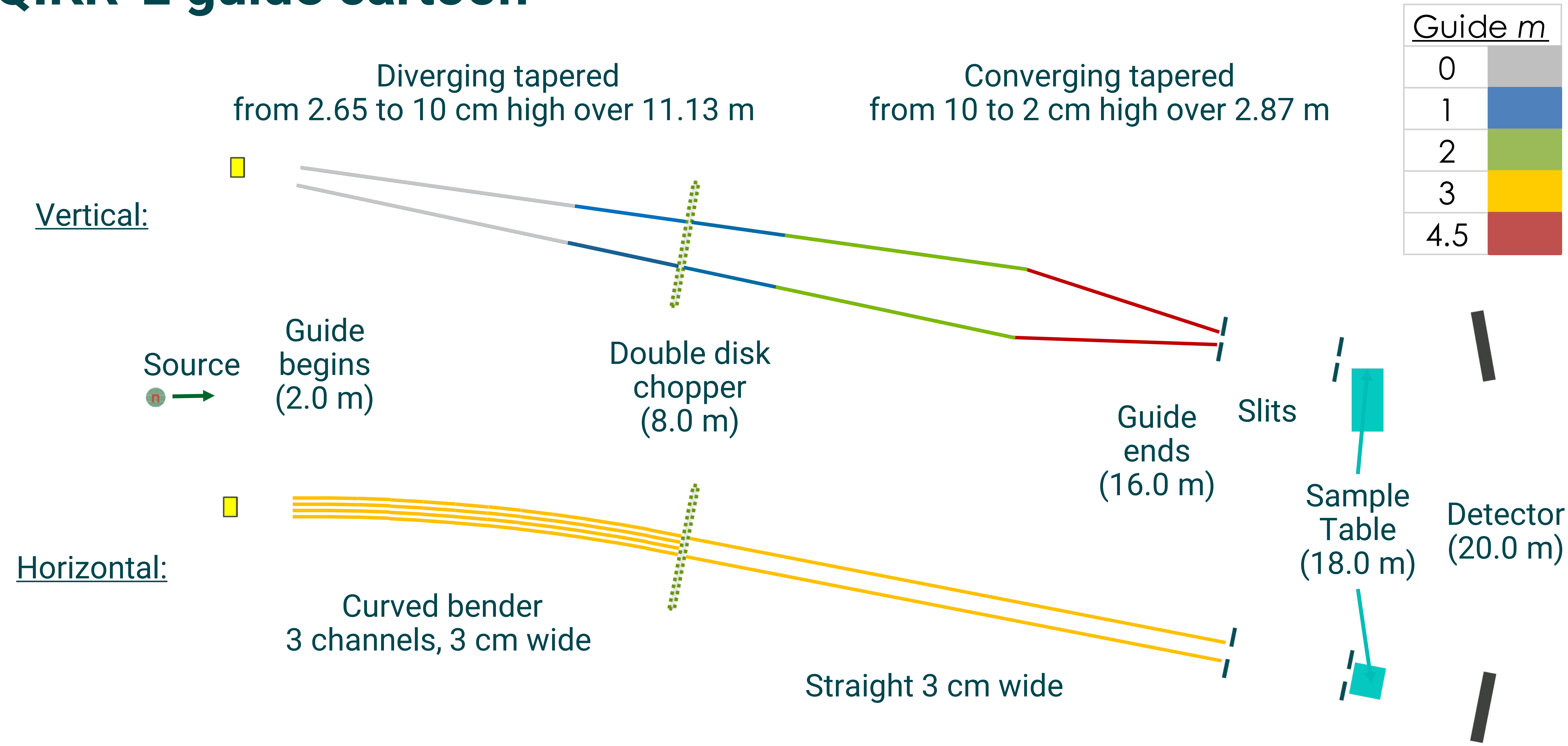
BB guides have 3 channels
(each has equal cross-sectional area)



BG and TG guides

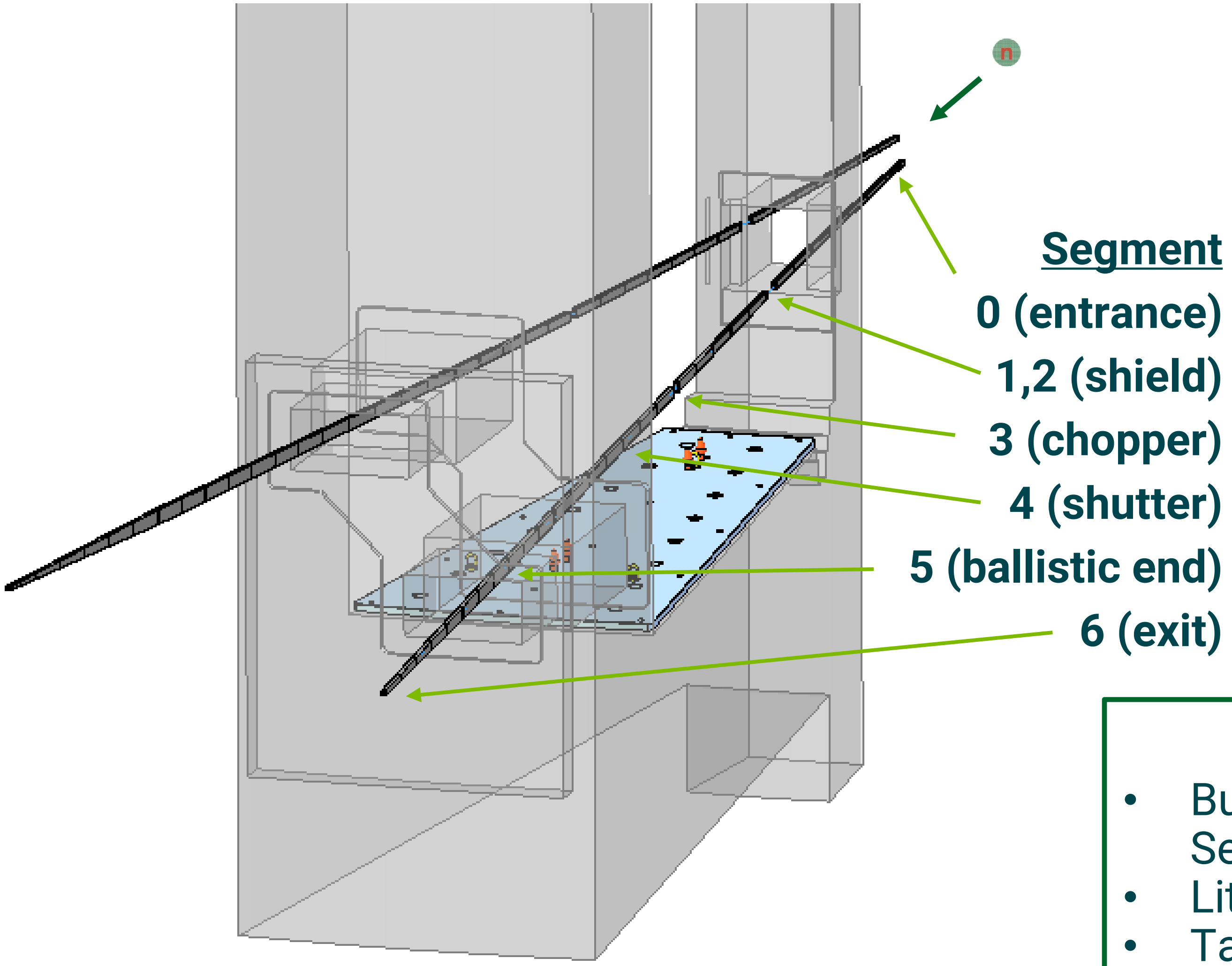


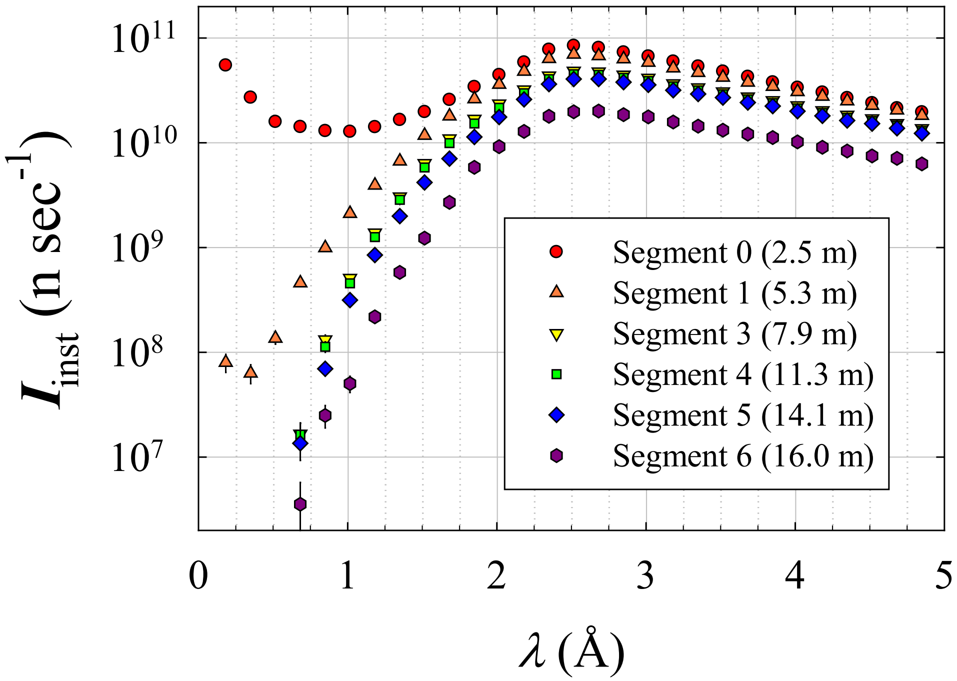
QIKR-L guide cartoon



The QIKR-L and QIKR-U guides have been optimized
to fulfill requirements at minimal cost in supermirror coating

Neutrons lost in monolith and bunker





A Tale of Loss

- Bulk of fast neutrons shed in Ballistic Bender (BB – Segments 1-2)
- Little loss in Ballistic Guide (BG – Segments 3-5)
- Tapered Guide (TG) trims unwanted thermal and cold neutrons (Segment 6)

→ **Shielding must mop up unused neutrons**

Outline

- QIKR, Briefly
- Unwanted Neutrons
  - Lost in monolith and bunker
  - **Lost in instrument cave**
- Summary

Guide system provides multiple beams

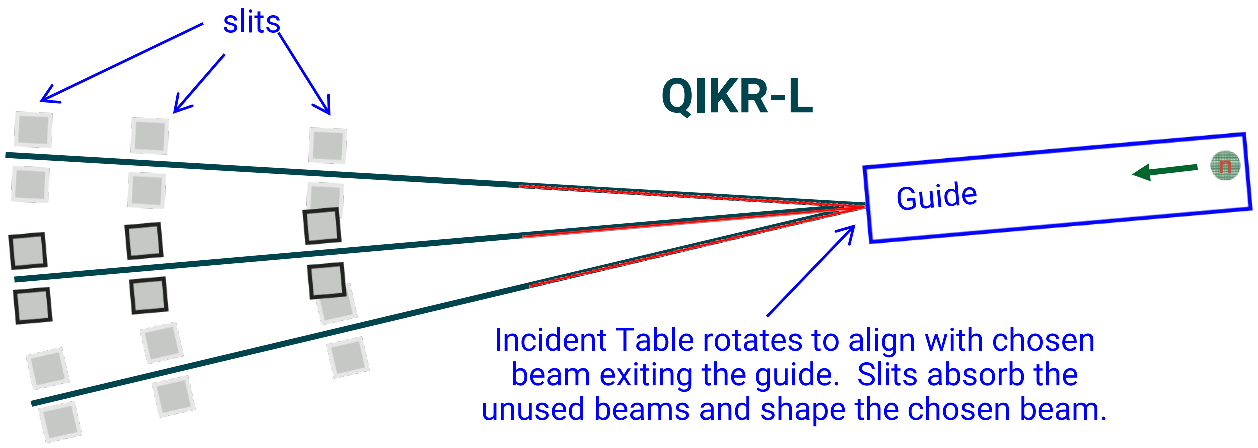
Characteristics

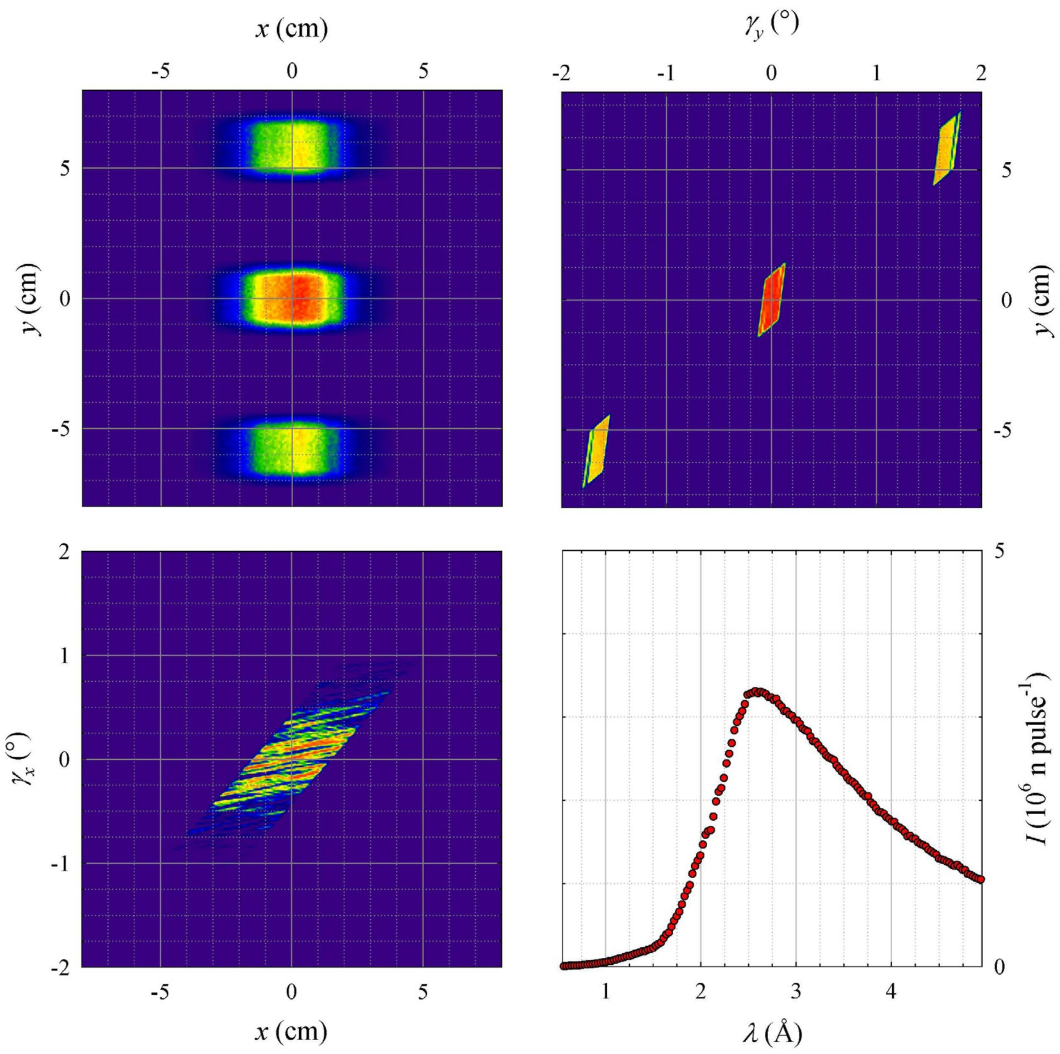
Three beams

…separated in space (y)

…and angle γ_y

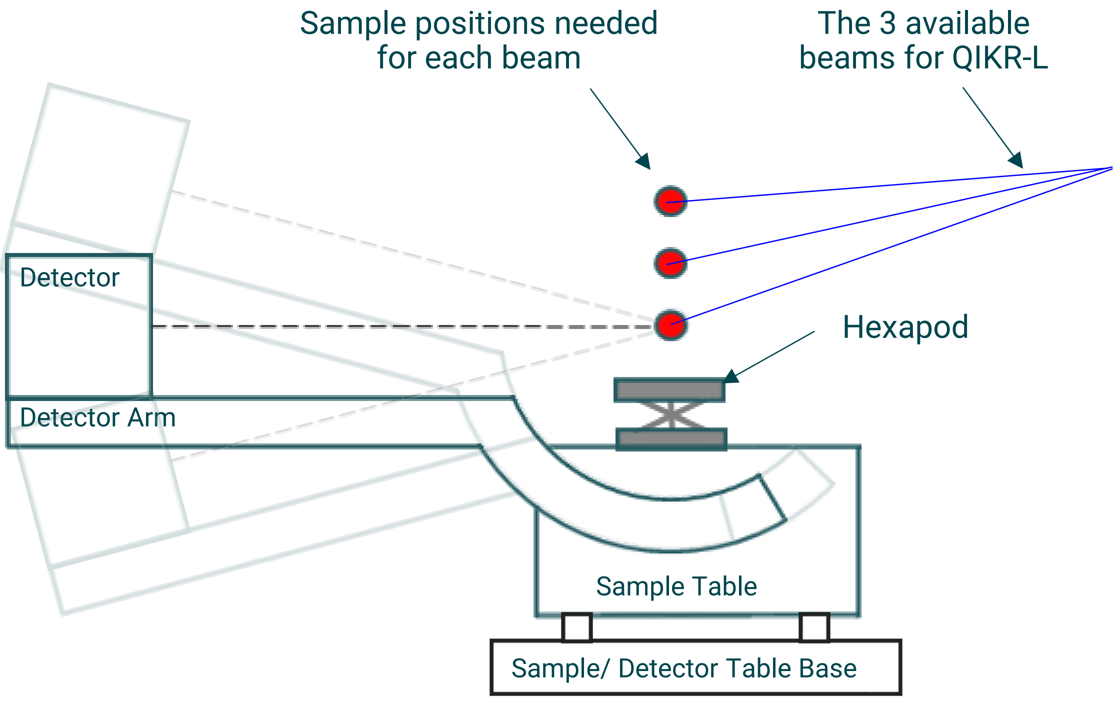
Select which to use in θ-θ geometry to span needed Q range





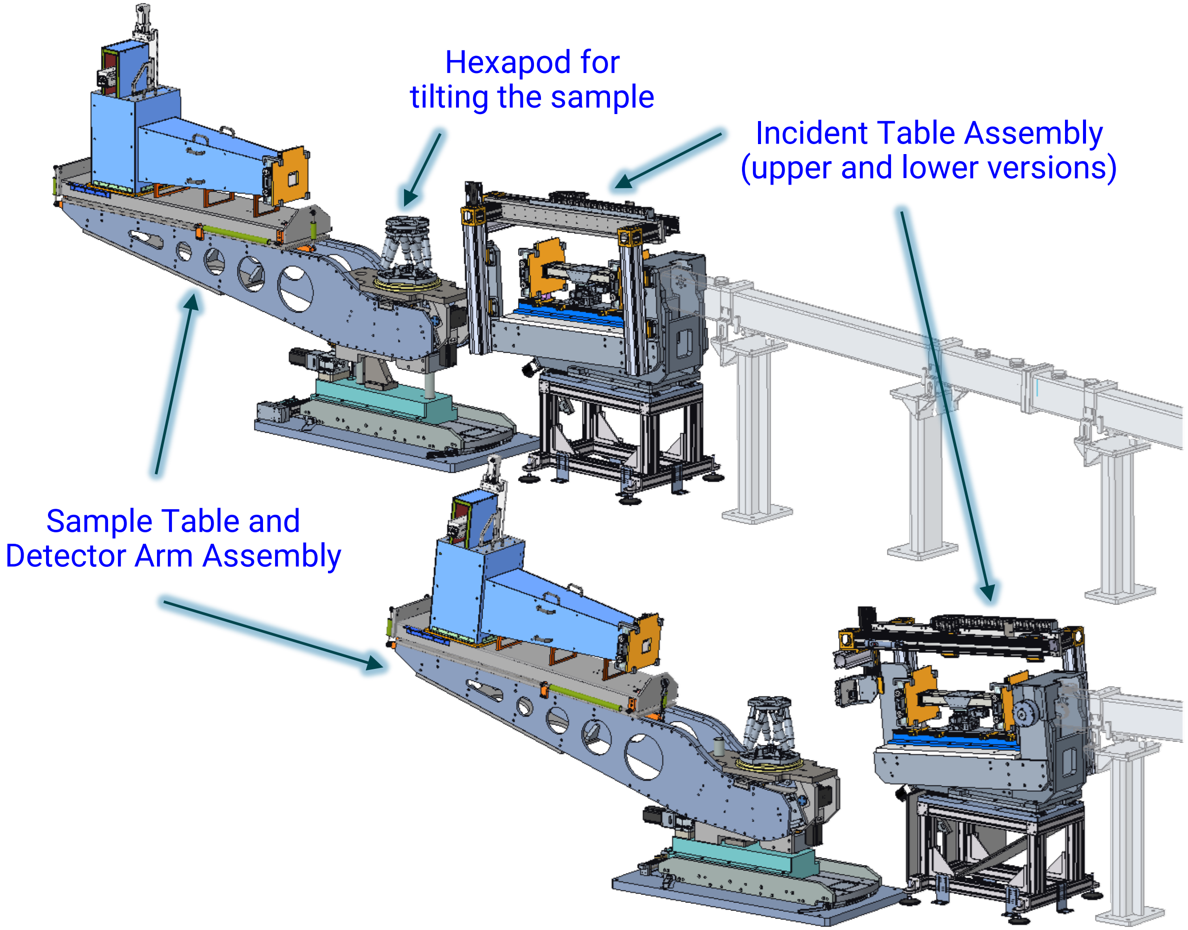
(QIKR-L McStas simulation)

QIKR end stations: beam selection and detector motion



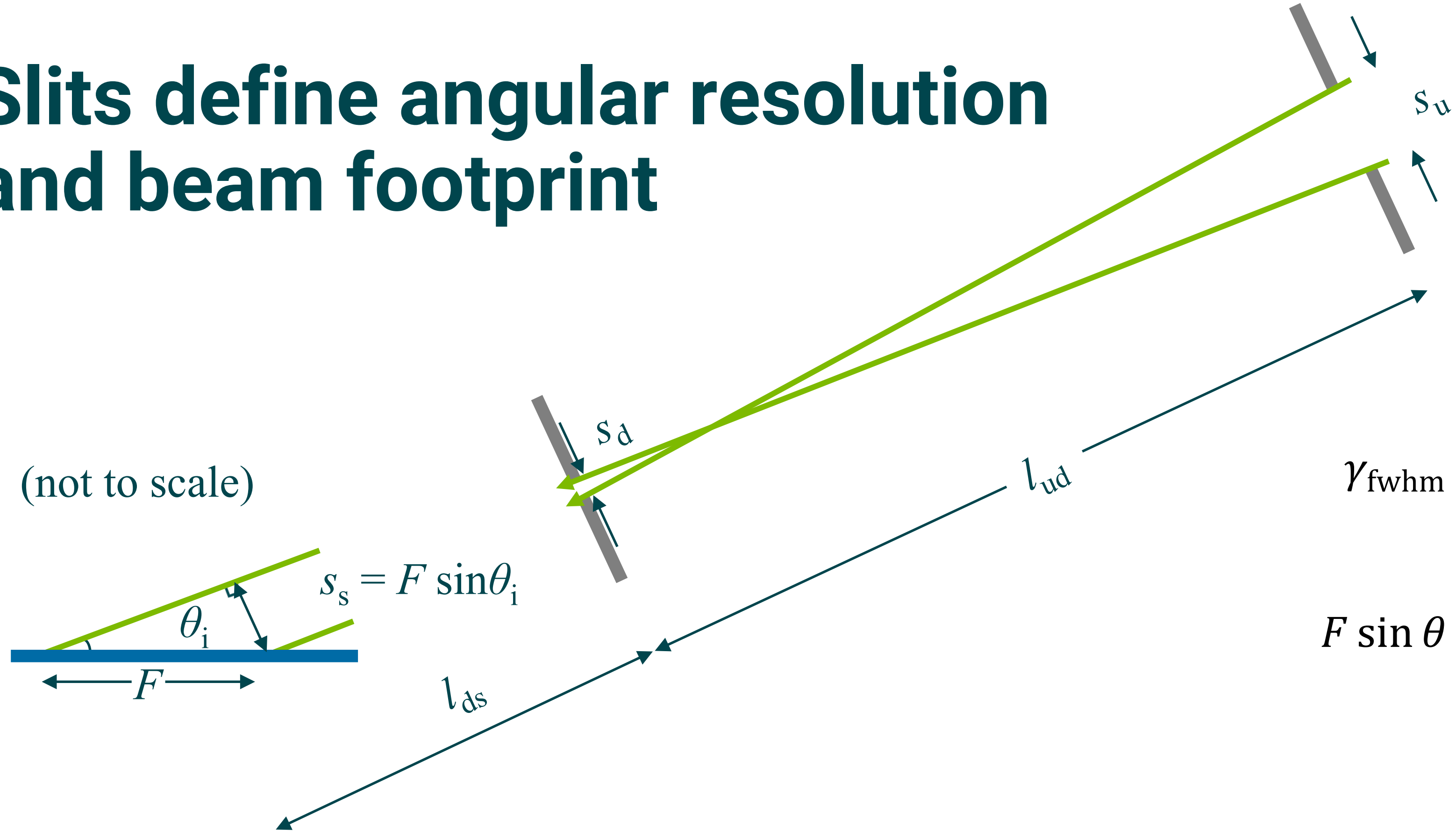
Detector Arm rotates about a horizontal *x* axis (out of the screen) passing through the sample center

Upper station (QIKR-U)



Lower station (QIKR-L)

Slits define angular resolution and beam footprint



$$\gamma_{fwhm} = \frac{1}{2}(\gamma_1 + \gamma_2) - \frac{1}{2}(\gamma_3 + \gamma_4) = \frac{s_u}{L_{ud}} \equiv \delta\theta$$

$$F \sin\theta \approx F\theta = s_s\theta = s_1 - s_3 = s_d + L_{ds}\frac{s_u + s_d}{L_{ud}}$$

$$s_u = L_{ud}\theta\left(\frac{\delta\theta}{\theta}\right)$$

=>

$$s_d = \frac{L_{ud}\theta[F - L_{ds}(\delta\theta/\theta)]}{L_{ud} + L_{ds}}$$

Slits s_u and s_d confine beam within footprint F at incident angle θ with angular divergence $(\delta\theta/\theta)$

→ All unwanted neutrons must be absorbed by shielding (slit blades and housings)

Useful data cannot be collected in the absence of collimating slits, so after commissioning they will remain in place

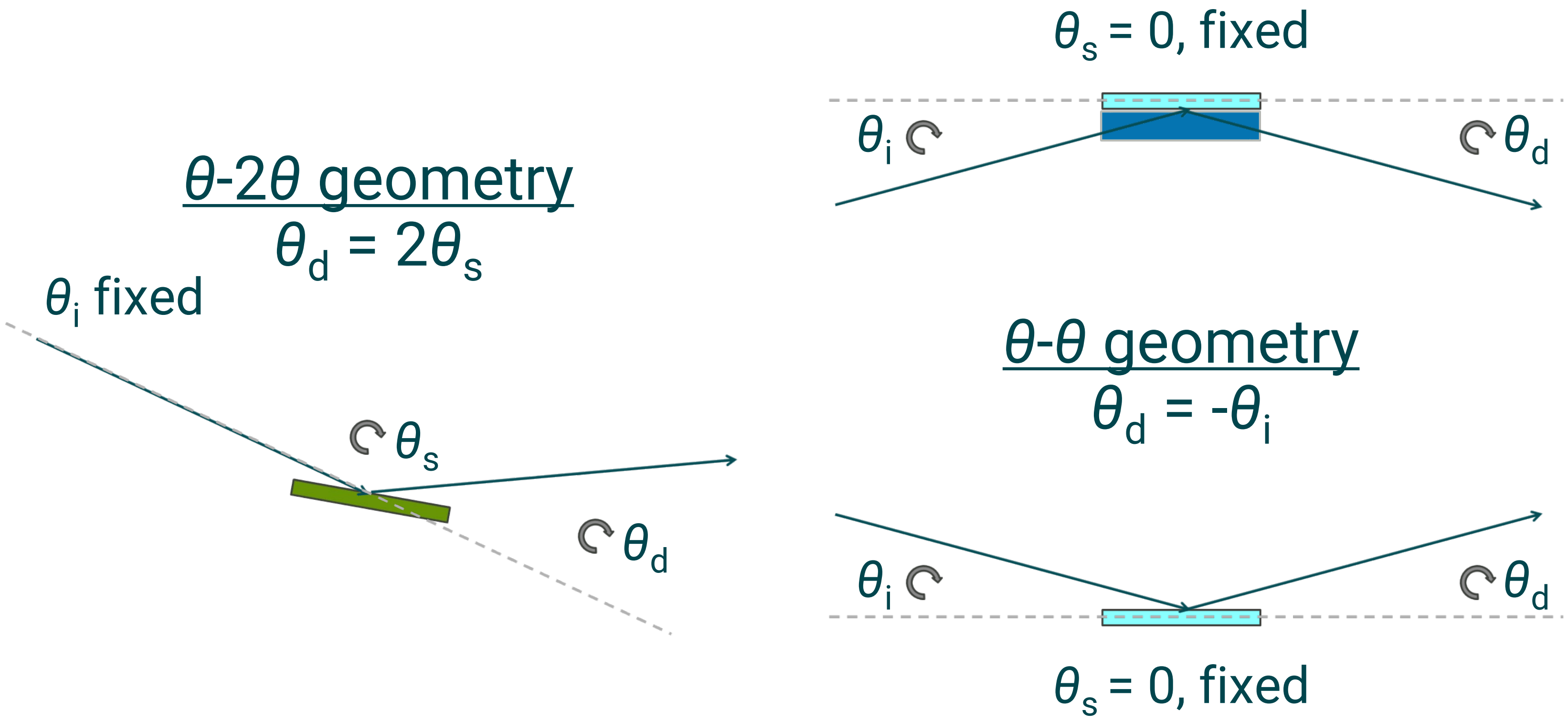
Operate in θ-2θ and θ-θ geometries

θ-2θ geometry

- Incident beam fixed
- Sample moves
- Detector moves

θ-θ geometry

- Incident beam varies
- Sample fixed
- Detector moves



Footprint calculator – maximum slits

Resolution

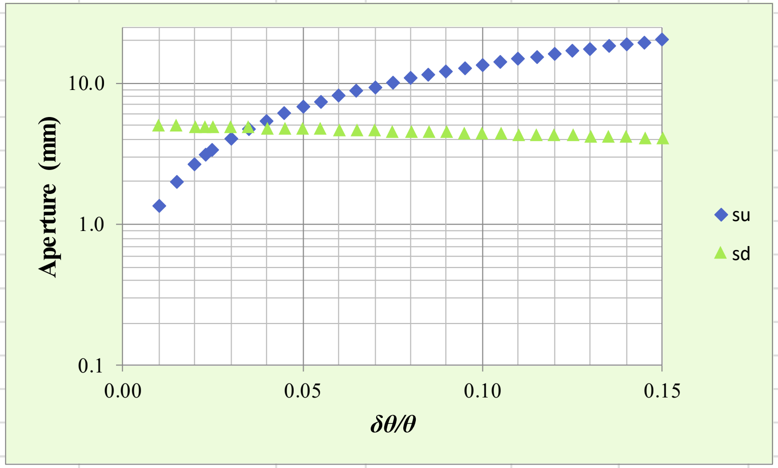
$0.02 < \delta\theta/\theta < 0.07$

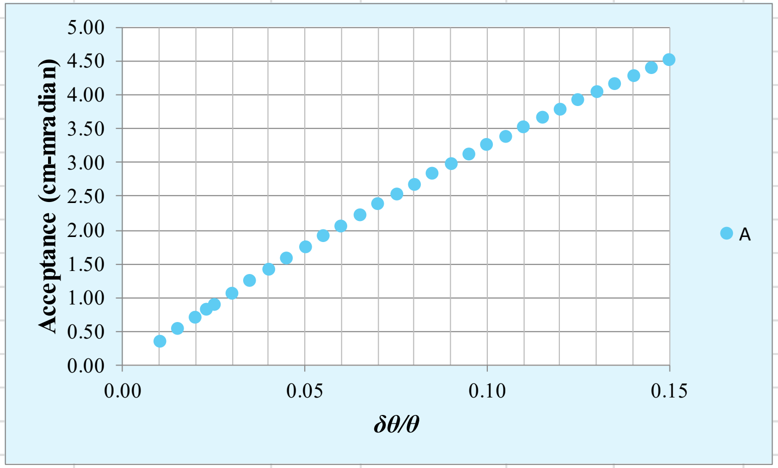
implies

$0.1\ \text{mm} < s < 10\ \text{mm}$

→ Maximum usable slit aperture is smaller than the fully open setting

	$\delta\theta/\theta$	s_u (mm)	s_d (mm)	A (cm-mradian)
θ (°)	0.010	1.36	5.11	0.372
4.17	0.015	2.05	5.08	0.554
L_{ud} (mm)	0.020	2.73	5.04	0.734
1875.0	0.023	3.14	5.02	0.841
L_{ds} (mm)	0.025	3.41	5.01	0.911
100.0	0.030	4.09	4.97	1.086
F (mm)	0.035	4.78	4.94	1.258
75.0	0.040	5.46	4.91	1.428
	0.045	6.14	4.87	1.595
	0.050	6.82	4.84	1.760
	0.055	7.51	4.80	1.922
	0.060	8.19	4.77	2.082
	0.065	8.87	4.73	2.239
	0.070	9.55	4.70	2.394
	0.075	10.23	4.66	2.546
	0.080	10.92	4.63	2.695
	0.085	11.60	4.59	2.843
	0.090	12.28	4.56	2.987
	0.095	12.96	4.53	3.129
	0.100	13.65	4.49	3.269
	0.105	14.33	4.46	3.406
	0.110	15.01	4.42	3.540
	0.115	15.69	4.39	3.672
	0.120	16.38	4.35	3.802
	0.125	17.06	4.32	3.929
	0.130	17.74	4.28	4.053
	0.135	18.42	4.25	4.175
	0.140	19.10	4.21	4.295
	0.145	19.79	4.18	4.411
	0.150	20.47	4.15	4.526



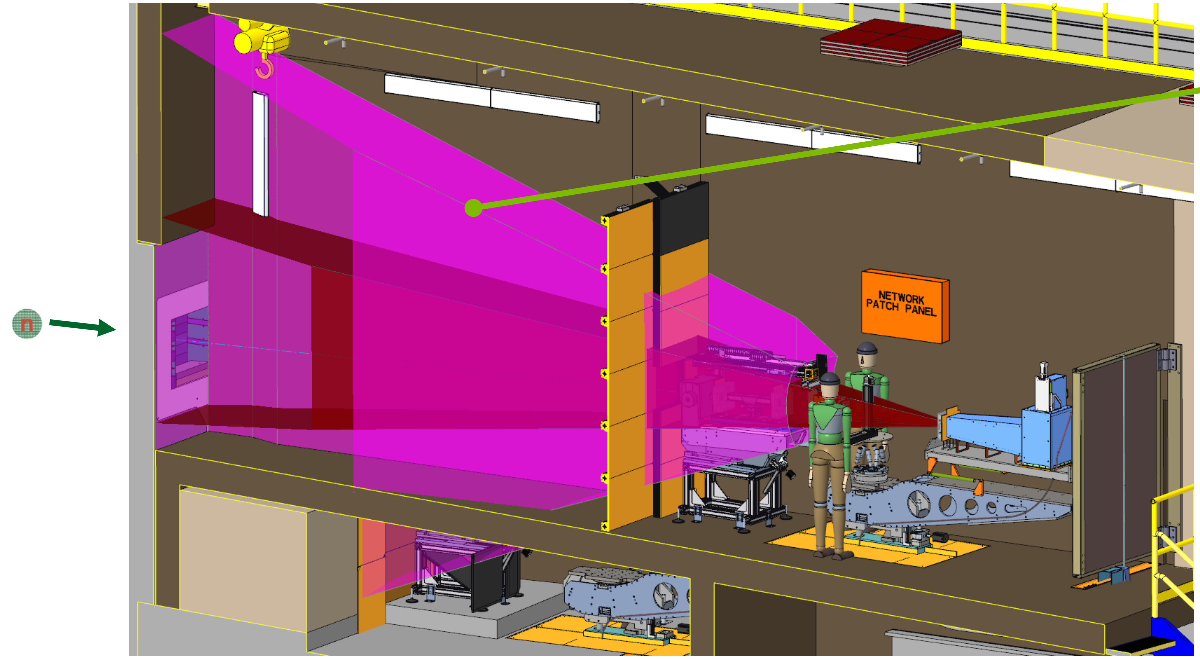


Detector sensitivity to unwanted neutrons (background)

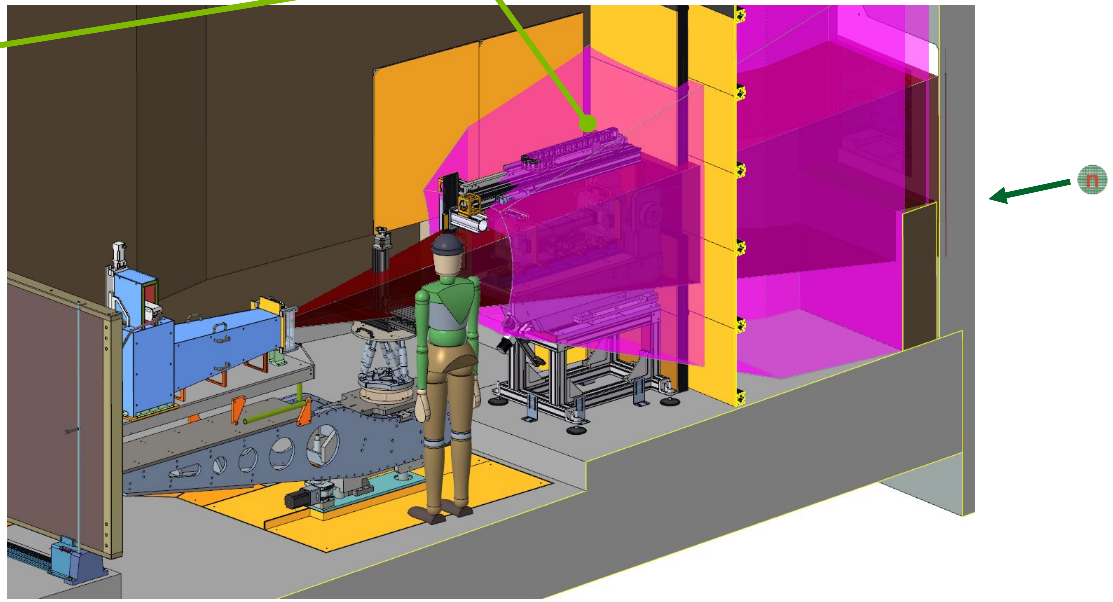
- Personnel safety is a necessary but not sufficient function of the shielding (the one investigated by neutronics analysis)
- Detector sensitivity to unwanted neutrons is the other function (**not** investigated by current neutronics analysis)
- Experience with the BL4B detector at SNS shows that using B_4C to block the detector's view of concrete surfaces is effective at reducing detector background

Backdrop must be dark

Every surface painted by the magenta cones is visible to the detector and should be shielded from view using B_4C (gold panels)



QIKR-U



QIKR-L

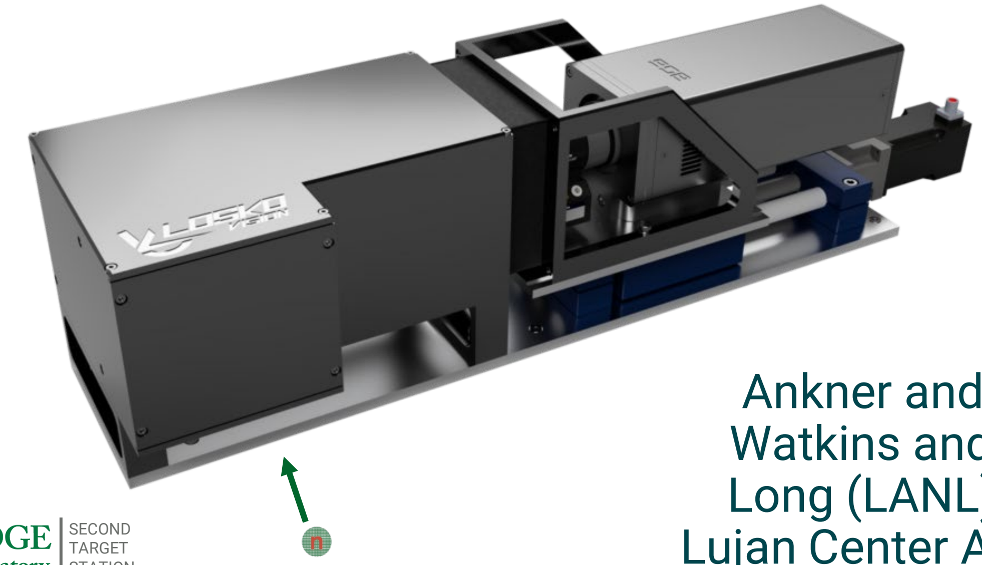
The backdrop of the sample, viewed by the detector, needs to be as dark as possible. The placement of B_4C shielding panels and additional wall-mounted shielding is dictated by this requirement.

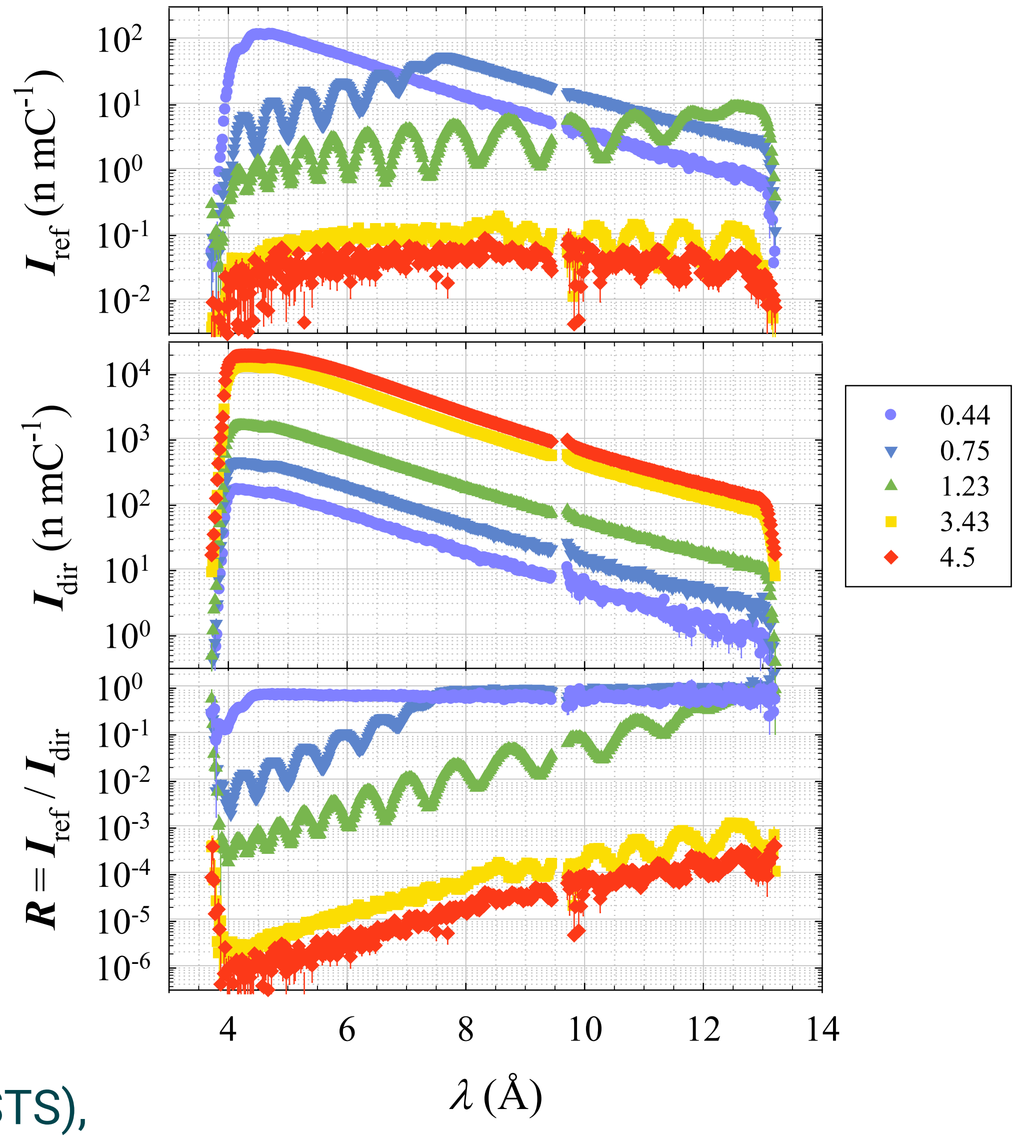
Detector assessment

Detector: Timepix3-based scintillator

- Equivalent performance to conventional ^{3}He detector
- Greater (>20×) count-rate capability
- Modular design – replaceable components
- Upgrade path to Timepix4

→ **Measuring R down to 10^{-7} requires low background**





Ankner and Khaplanov (STS), Watkins and Loyd (NScD), and Long (LANL) data collected at Lujan Center Asterix reflectometer

Define beam – reject even more neutrons

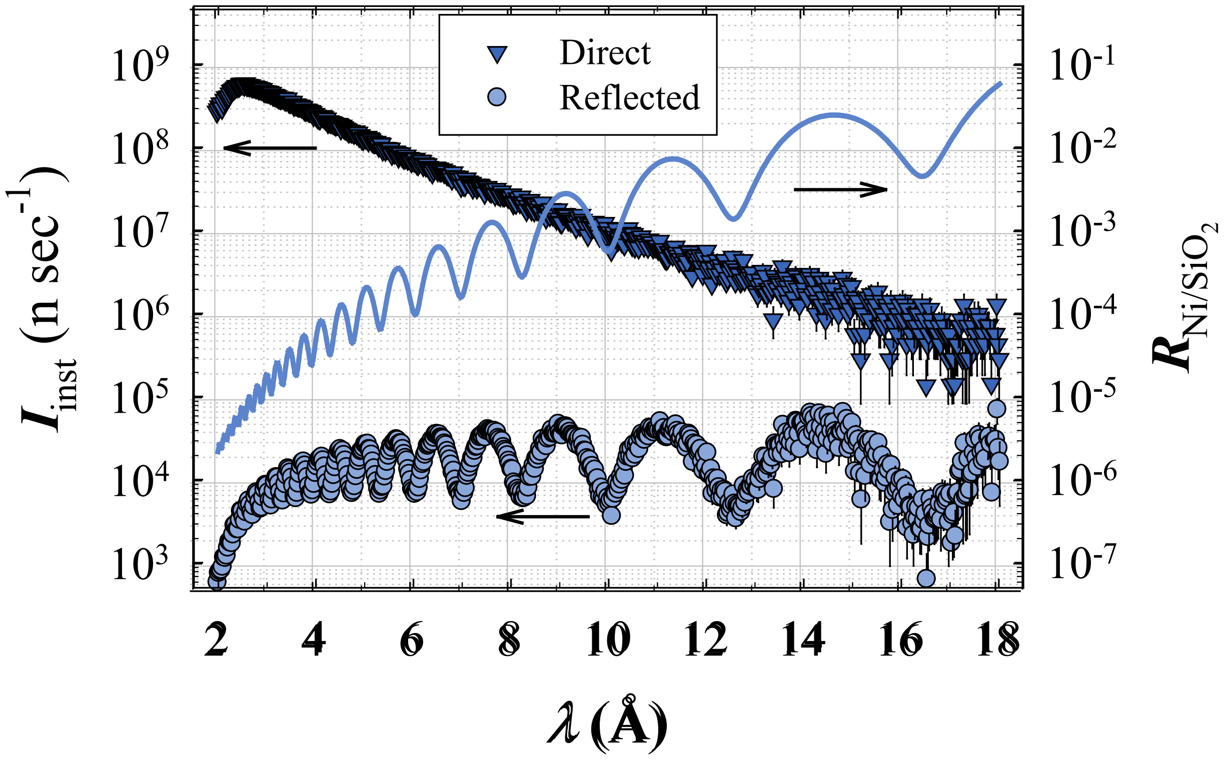
<u>Beam-defining slits</u>

- Select a satellite beam
- Collimate to define resolution and footprint
- Reduce intensity >67%

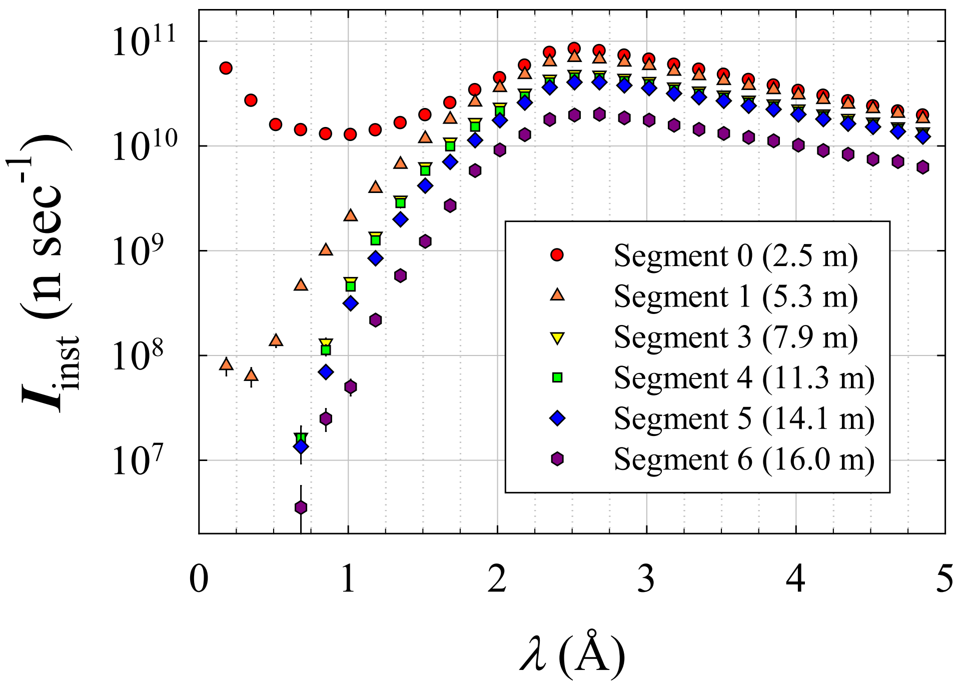
<u>Sample reflectivity</u>

- Further reduction of intensity by factor of 10^{-7}-1 depending on λ

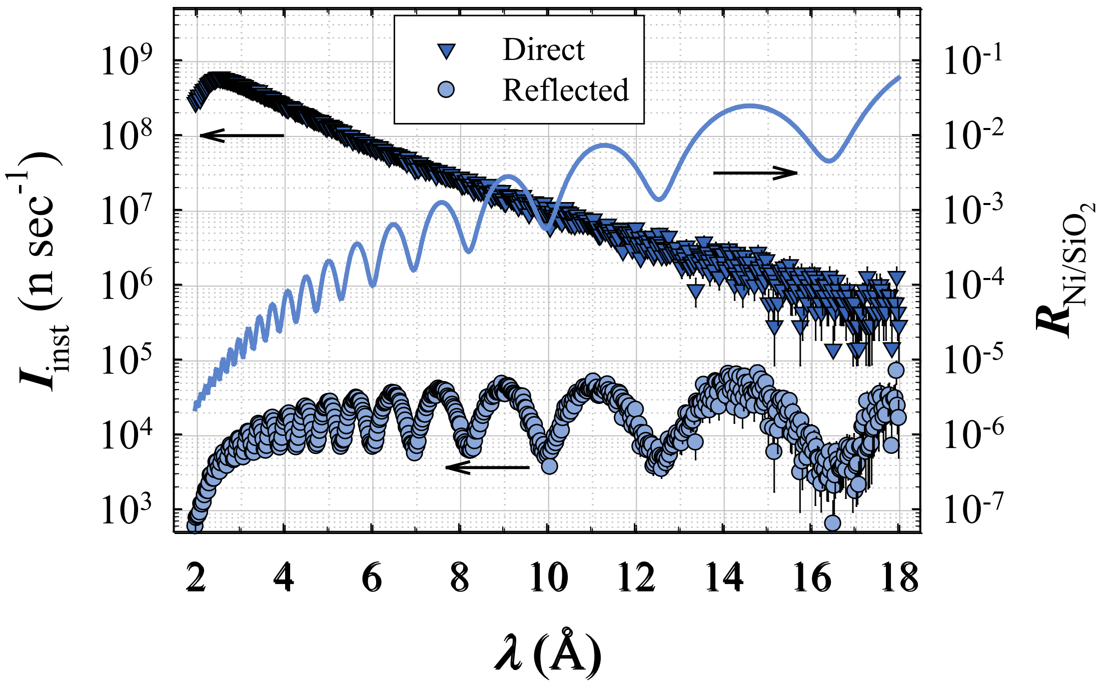
→ Shielding in cave must mop up unused thermal and cold neutrons



There are a lot of neutrons to absorb



Fast neutrons in the monolith and bunker



Thermal and cold neutrons in the instrument cave

OAK RIDGE National Laboratory | SECOND TARGET STATION

Outline

- QIKR, Briefly
- Unwanted Neutrons
  - Lost in monolith and bunker
  - Lost in instrument cave
- **Summary**

Summary

- The curvature of the QIKR guides causes high energy neutrons to depart the guide and enter the bunker→shielding is needed for biological safety and to prevent those neutrons from entering the cave & creating excessive background
- The tapering at the end of the QIKR guide causes large neutron loss inside the cave→shielding needs to absorb those neutrons
- The tapered guide creates multiple beams exiting the guide→slits select the desired beam and shield (block) the rest
  - There is not a reasonable scenario where the slits would be removed before turning on the beam→no useful data can be collected in that state
- Additional shielding is needed to minimize unwanted neutrons entering the detector
  - An effective solution on BL4B was to have the detector view panels of ZHIP mix (B_4C) rather than concrete surfaces→the same will be done on QIKR, though neutronic analysis to confirm its effectiveness has not yet been done

Thanks

ORNL STS Design Team

- John Ankner
- Danielle Wilson
- Kursat Bekar
- Ryan Butz
- Joe Griffith
- Rudy Thermer
- Anton Khaplanov

Footprint calculator – maximum slits

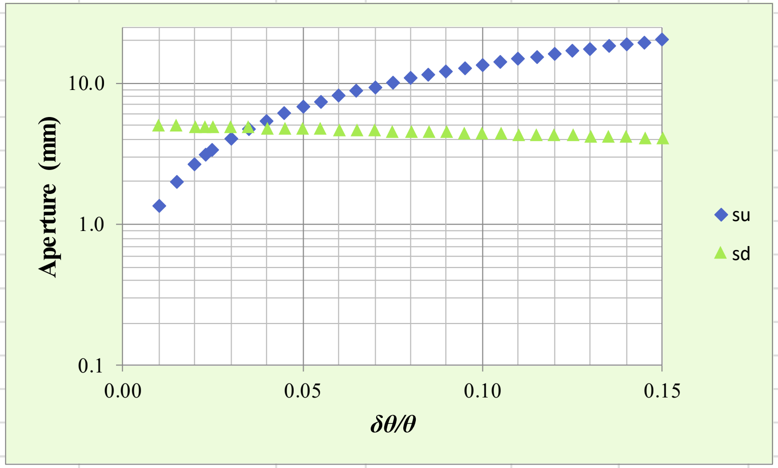
<u>Resolution</u>

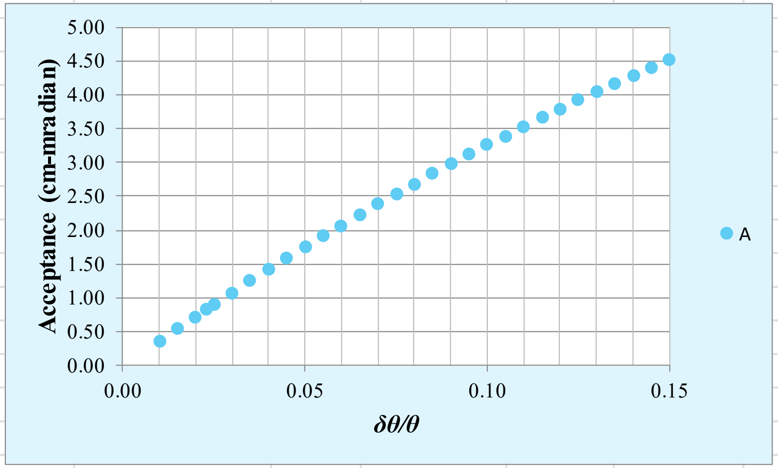
$0.02 < \delta\theta/\theta < 0.07$

implies

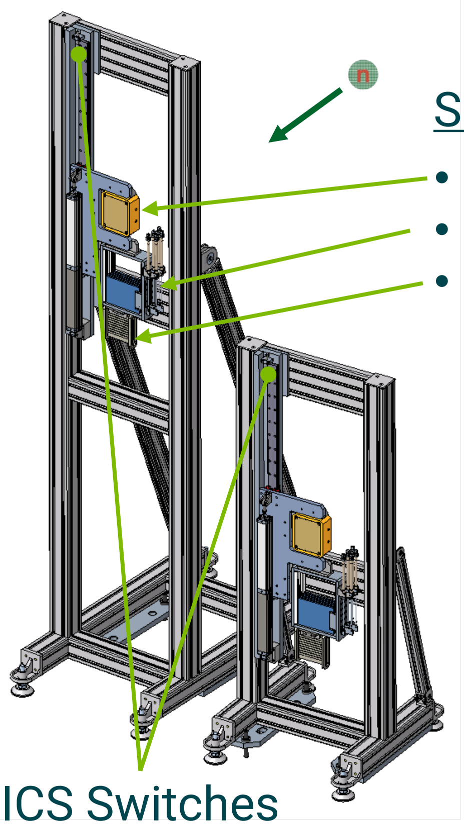
0.1 mm $< s < 10$ mm

	$\delta\theta/\theta$	s_u (mm)	s_d (mm)	A (cm-mradian)
θ (º)	0.010	1.36	5.11	0.372
4.17	0.015	2.05	5.08	0.554
L_{ud} (mm)	0.020	2.73	5.04	0.734
1875.0	0.023	3.14	5.02	0.841
L_{ds} (mm)	0.025	3.41	5.01	0.911
100.0	0.030	4.09	4.97	1.086
F (mm)	0.035	4.78	4.94	1.258
75.0	0.040	5.46	4.91	1.428
	0.045	6.14	4.87	1.595
	0.050	6.82	4.84	1.760
	0.055	7.51	4.80	1.922
	0.060	8.19	4.77	2.082
	0.065	8.87	4.73	2.239
	0.070	9.55	4.70	2.394
	0.075	10.23	4.66	2.546
	0.080	10.92	4.63	2.695
	0.085	11.60	4.59	2.843
	0.090	12.28	4.56	2.987
	0.095	12.96	4.53	3.129
	0.100	13.65	4.49	3.269
	0.105	14.33	4.46	3.406
	0.110	15.01	4.42	3.540
	0.115	15.69	4.39	3.672
	0.120	16.38	4.35	3.802
	0.125	17.06	4.32	3.929
	0.130	17.74	4.28	4.053
	0.135	18.42	4.25	4.175
	0.140	19.10	4.21	4.295
	0.145	19.79	4.18	4.411
	0.150	20.47	4.15	4.526





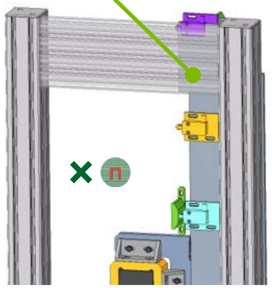
In-bunker components

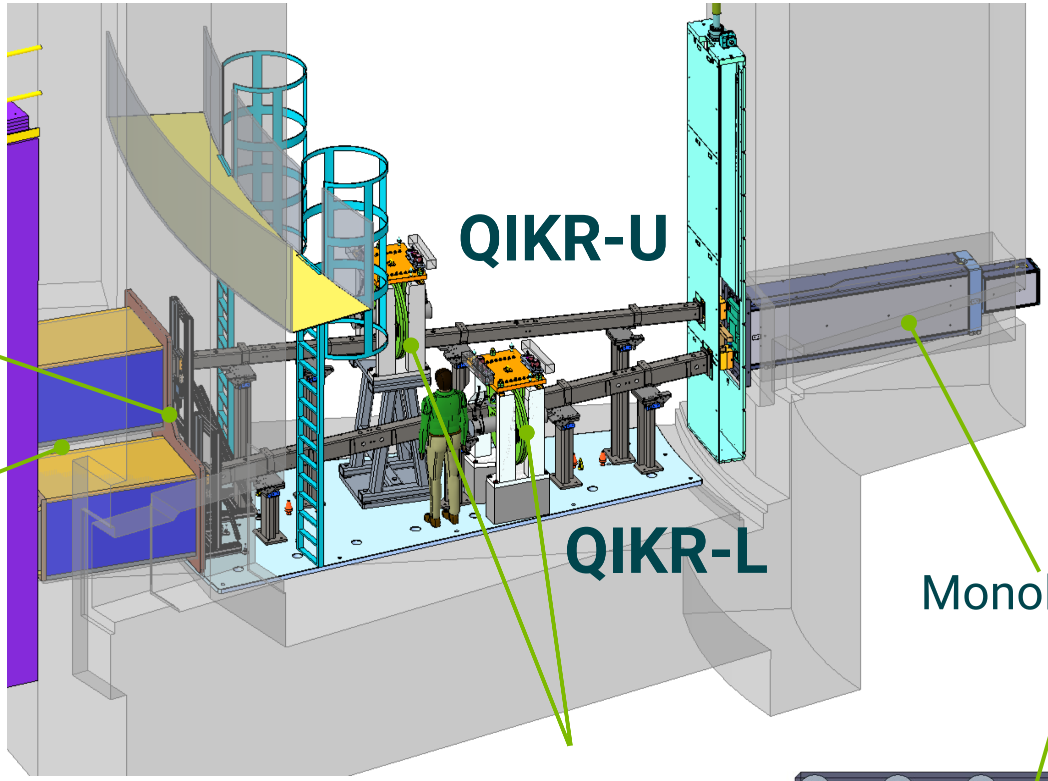


Shutter assemblies

- B_4C / W shutter
- Attenuator deck
- Beam monitor

ICS Switches

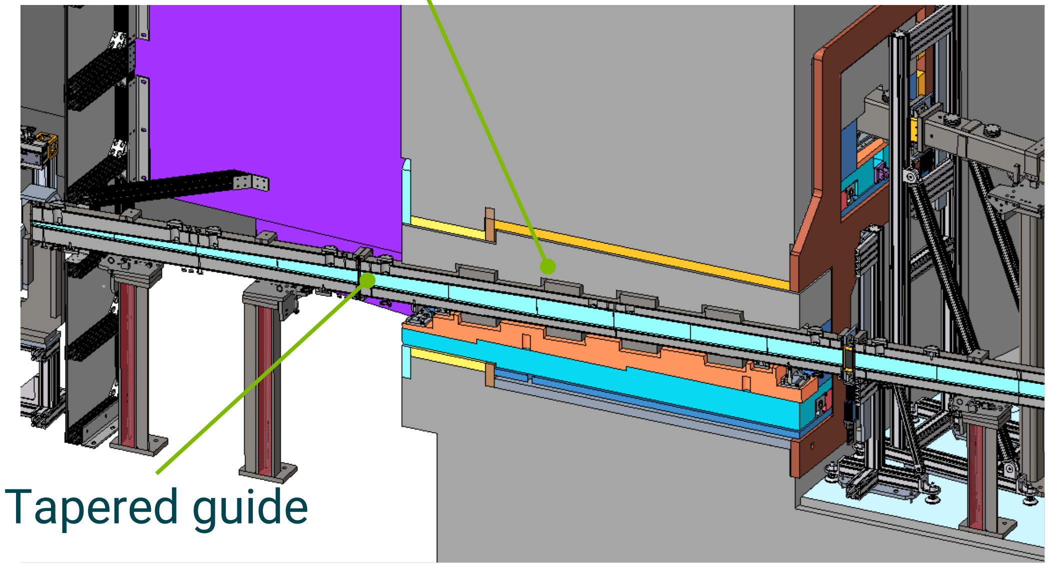




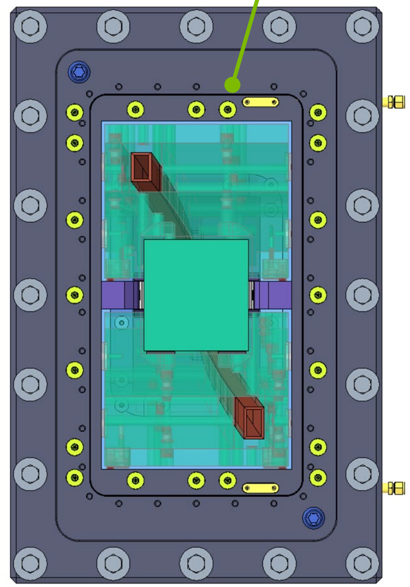
Bunker inserts

Monolith insert

Bandwidth choppers

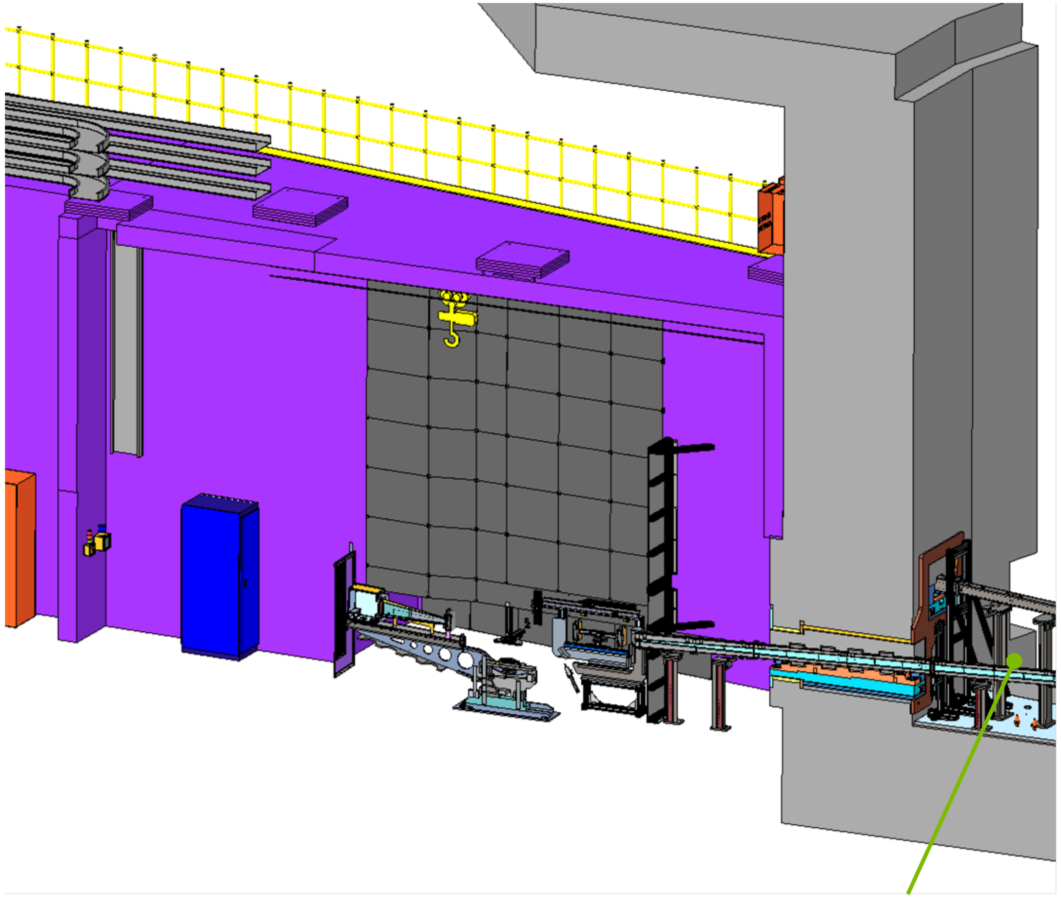


Tapered guide



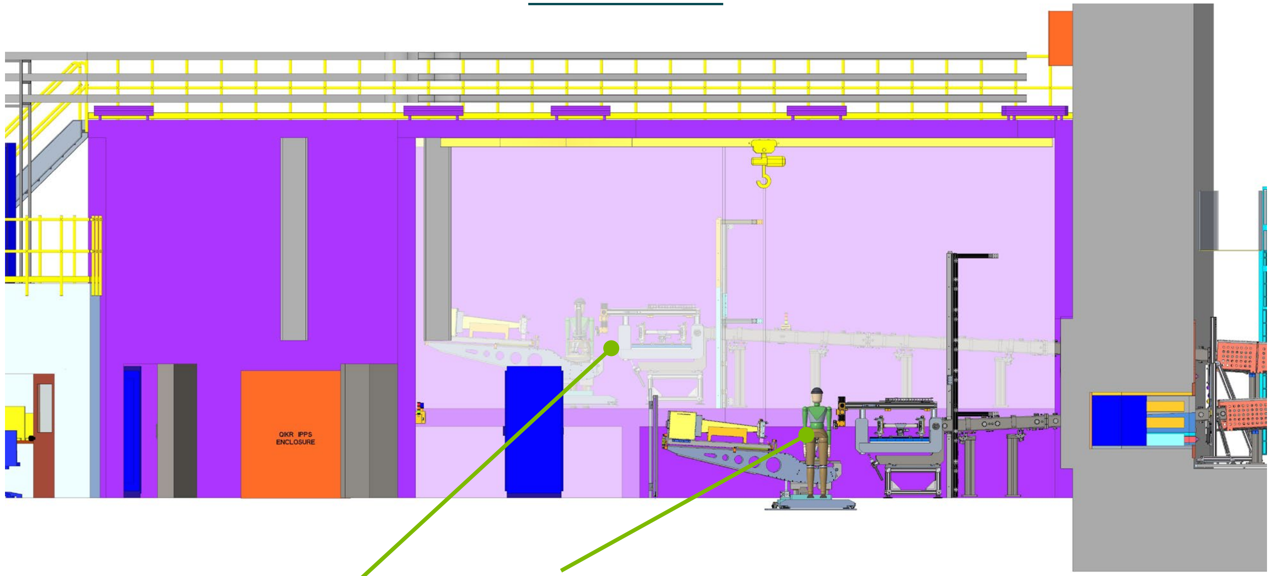
End-station caves

Isometric



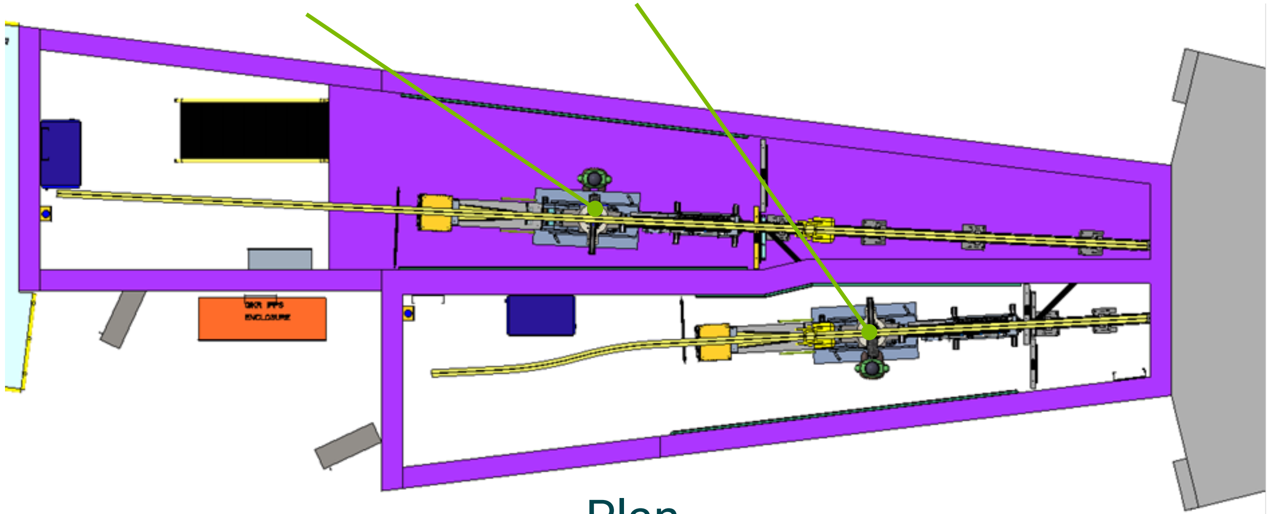
Bunker

Elevation



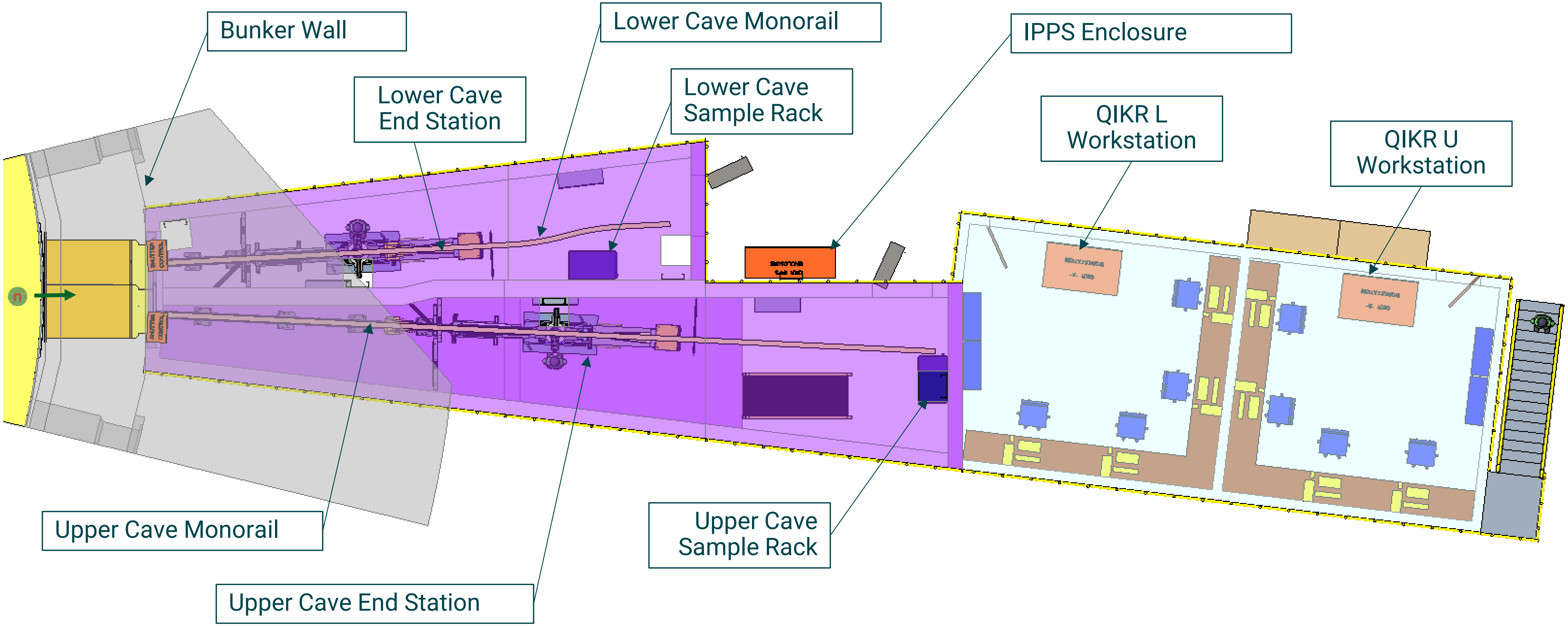
QIKR-L ← 20 m

QIKR-U ← 24 m



Plan

QIKR Caves & User Hutches – plan view



McStas Analysis

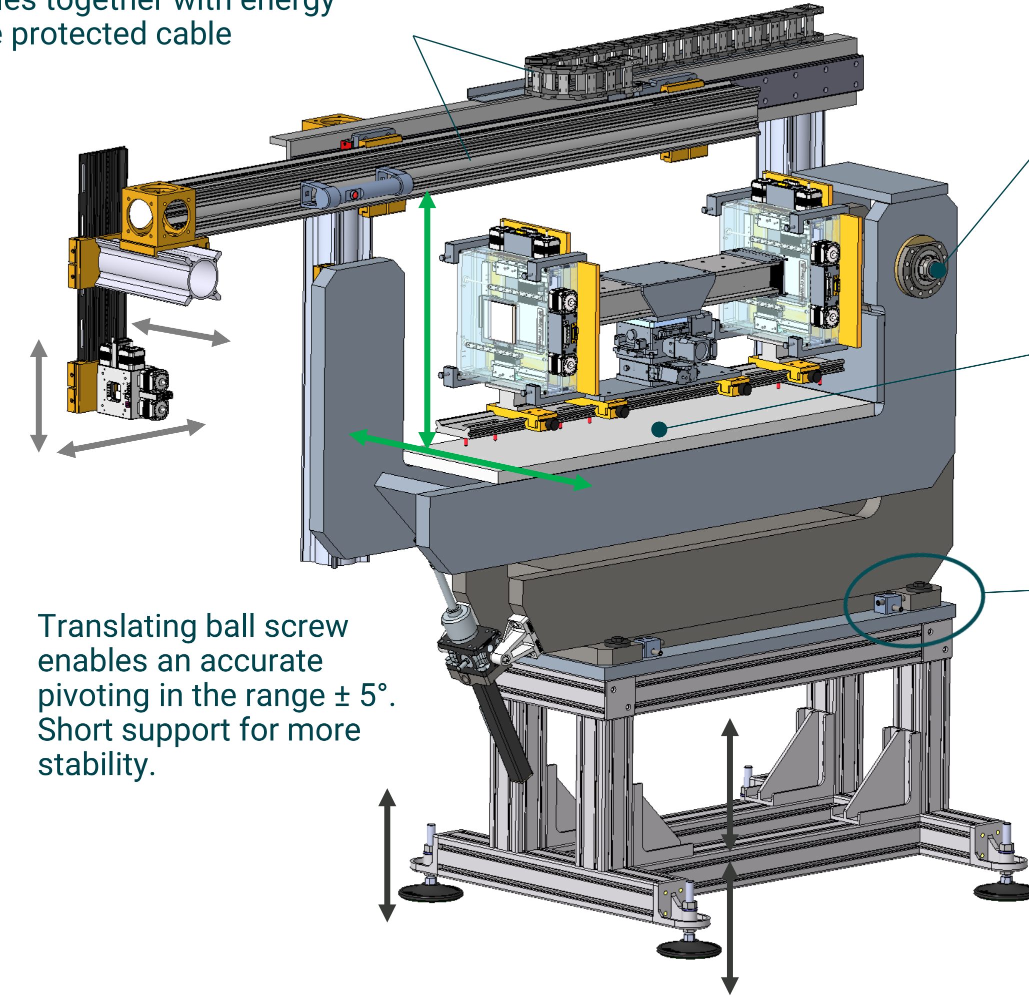
- McStas can tell the neutrons leave the guide, but can't tell where they go afterward… the shielding has to mop up those neutrons
- MCNP analysis agrees with McStas to within 10% if the same source is used in each
  - Therefore MCNP reflects low-energy neutrons correctly
- McStas also matches Creo geometry

Incident Table – holds slits and optics

Preliminary design of an incident table for QIKR

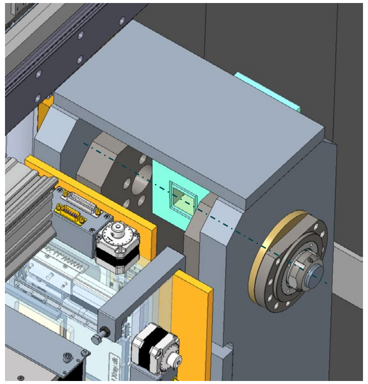
Hollow profiles together with energy chain enable protected cable installation.

Manually adjustable slit position with safety brake in *z*-direction.



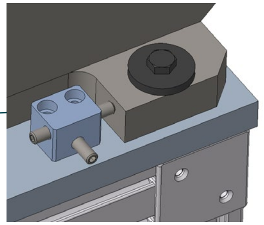
Translating ball screw enables an accurate pivoting in the range ± 5°. Short support for more stability.

The axis of rotation ideally lies on the face and the symmetry plane of the neutron guide.



A rigid bearing ensures precise alignment of the slits.

A platform open to the sides, with sufficient distance to the beam line, offers flexible installation space for future installations.



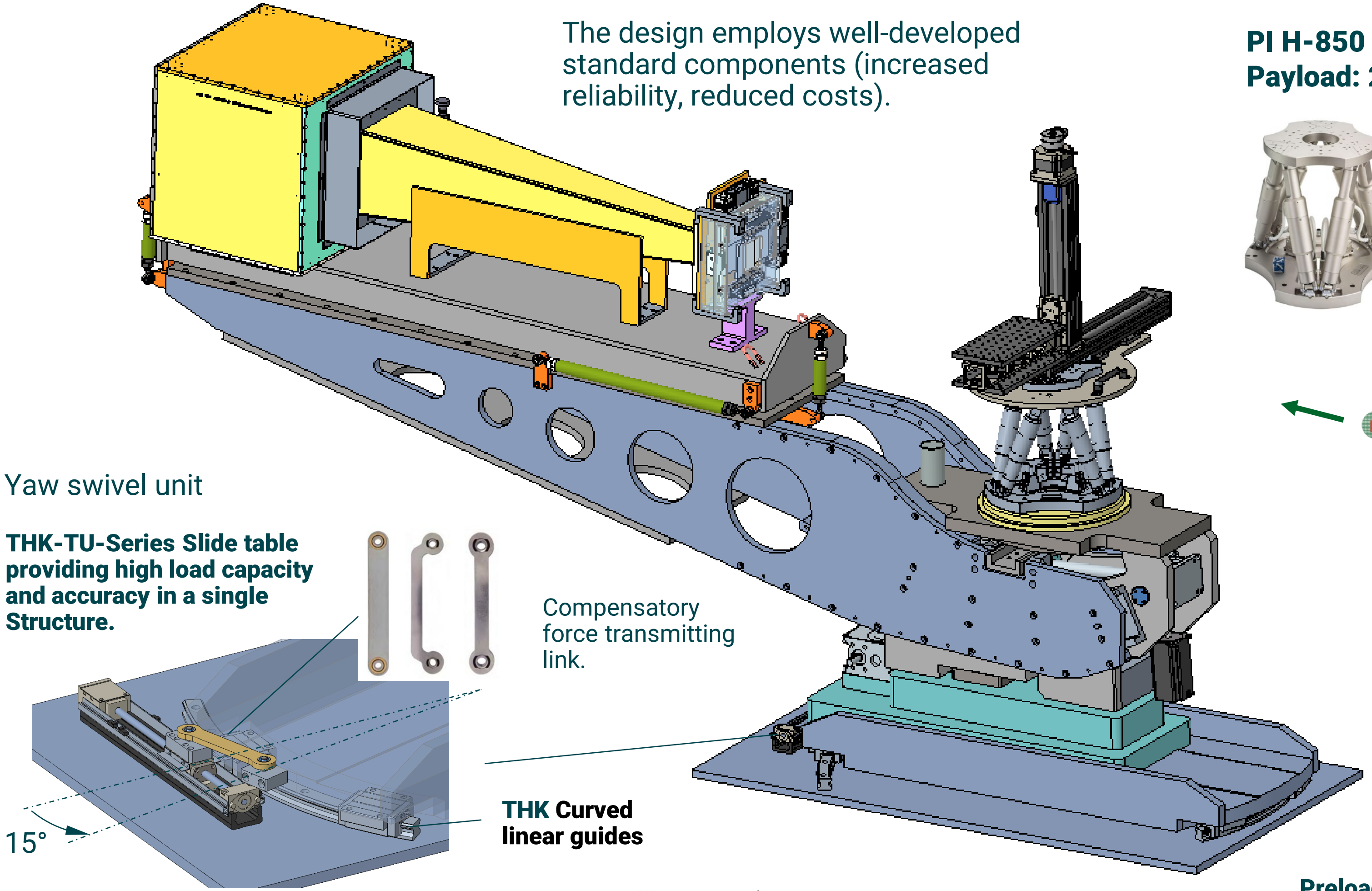
Adjustability in the *xz* plane.

Adjustable machine feet with vibration absorbing pads.

[courtesy Rudy Thermer]

Sample Table and Detector Arm unit

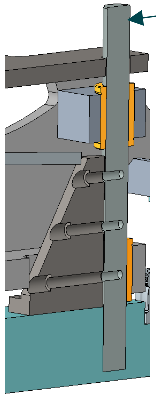
The design employs well-developed standard components (increased reliability, reduced costs).



PI H-850 Hexapod
Payload: 250 kg

Hexapods offer six degrees of freedom of movement in the most compact space.

Robust guide system

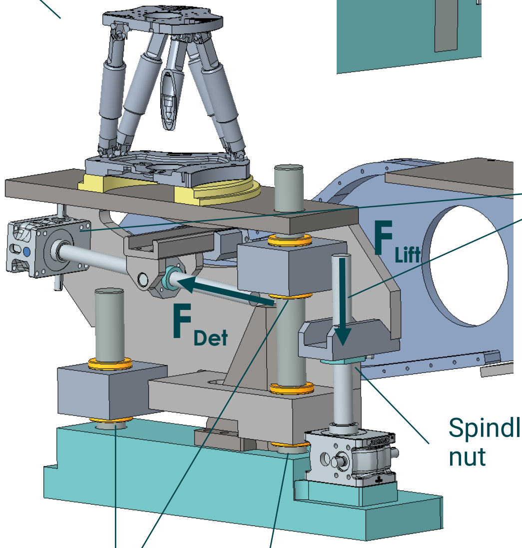


Ø 60 mm

Increased stiffness due to a free length Reduction of 50%.

ZIMM Screw Jack

Available with different load capacities i.e., various spindle sizes, gear ratios and accuracies.



Spindle nut

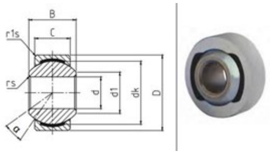
Yaw swivel unit

THK-TU-Series Slide table providing high load capacity and accuracy in a single Structure.

Compensatory force transmitting link.

THK Curved linear guides

Nadella GLK (NIRO)
Spherical-plain bearing
Radial clearance: 0 -10 μm!

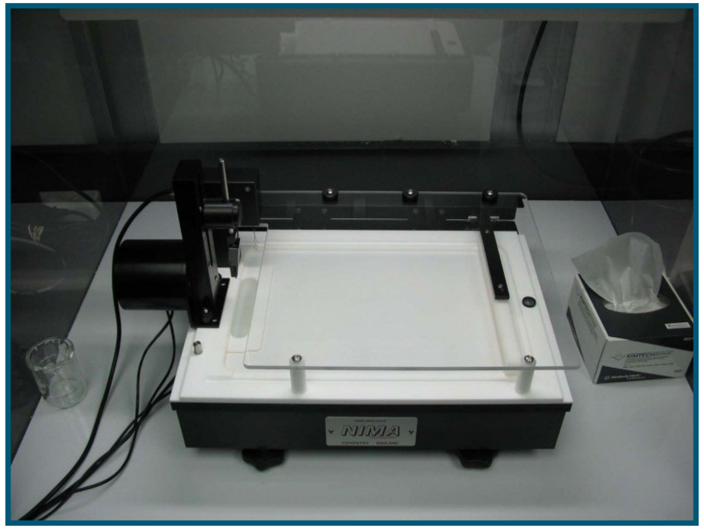


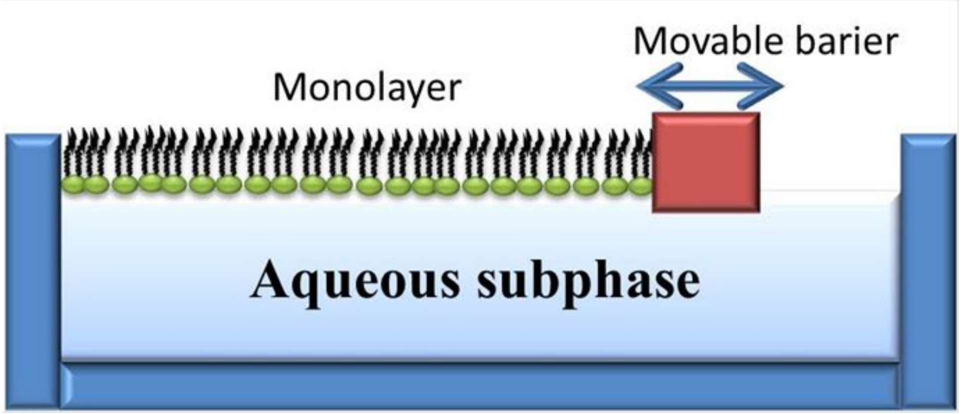
[courtesy Rudy Thermer]

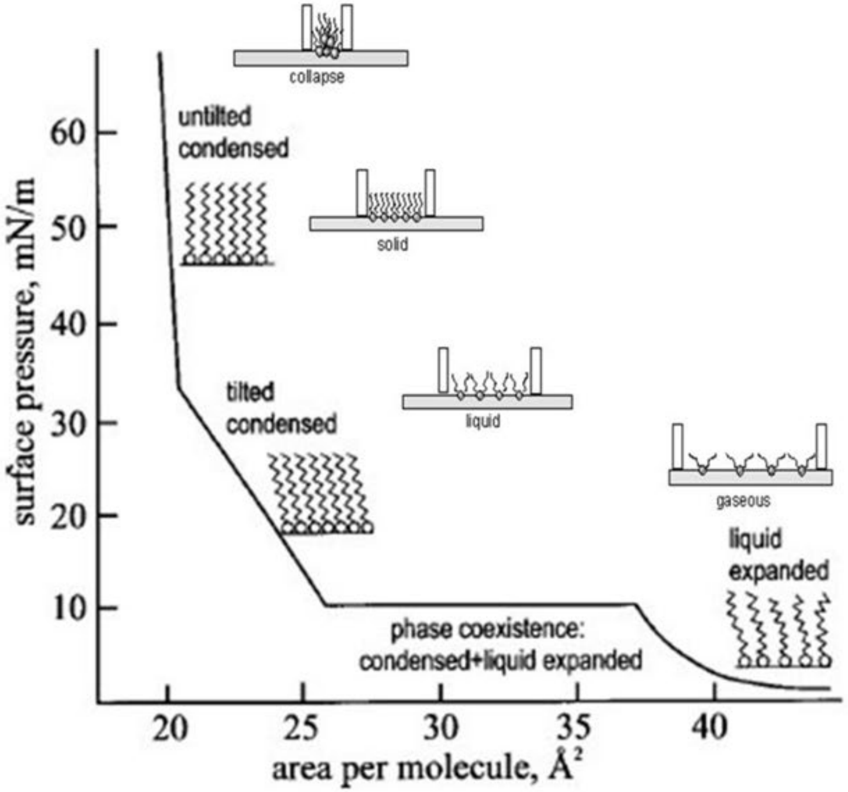
Preloaded linear ball bushings

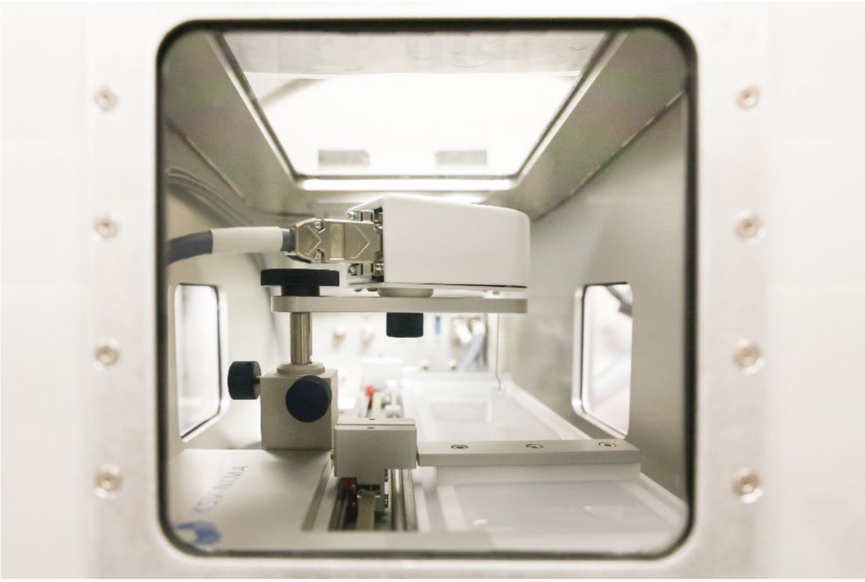
With an ideal load-bearing arrangement in relation to the spindle lifting nut.

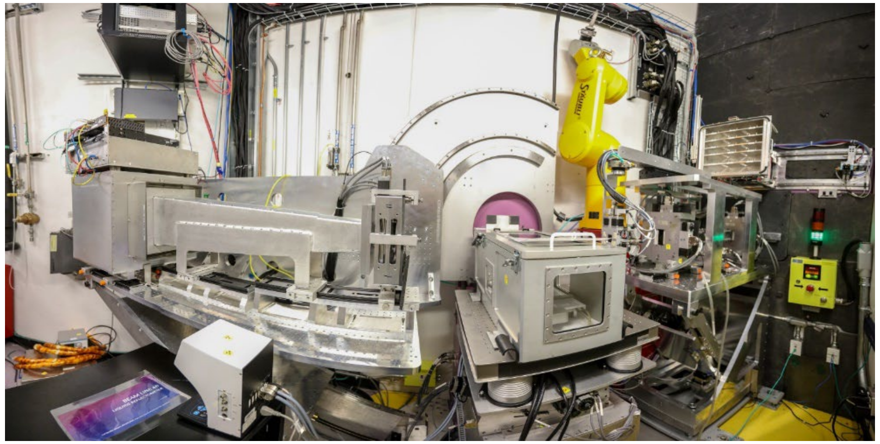
Create a layer: Langmuir trough









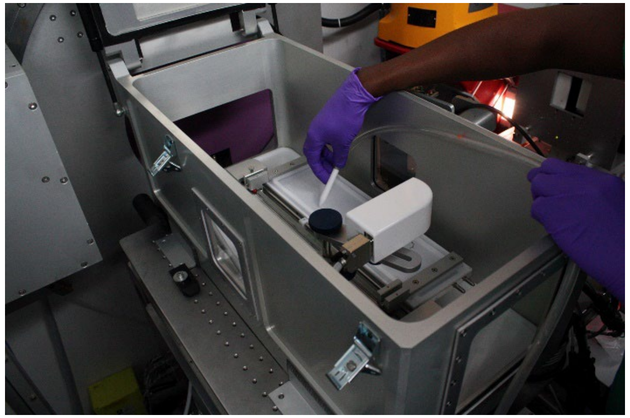


Biological Membrane Studies Conducted at Liquids Reflectometer

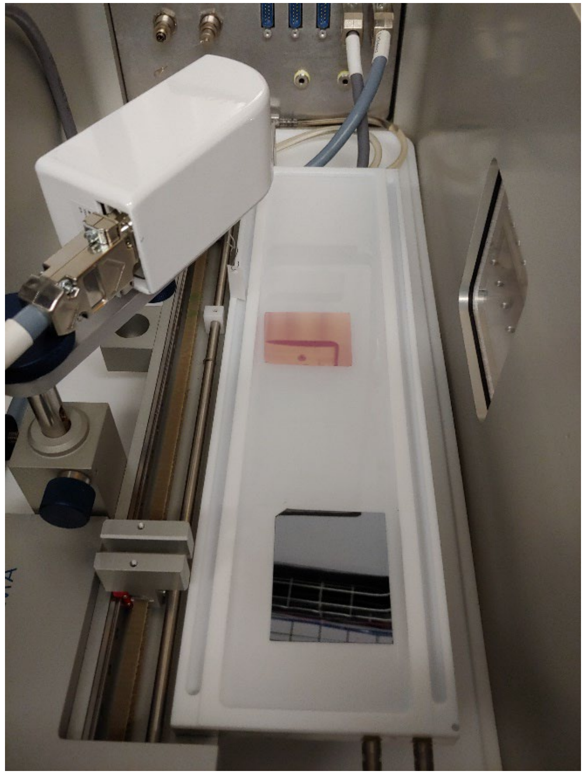
- Lipid membranes form the boundary between cells and the outside world
- Membranes (e.g. analogues of lung cells) are spread on a water surface or a solid (e.g. silicon) support
- Viral proteins and potential drugs are introduced into the water below the film
- Neutrons see the nano-scale rearrangements of the protein relative to the membrane under different conditions
- These rearrangements reveal protein function

Prepare DPPC film and measure NR

- Dual barrier KSV NIMA frame assembly
- Three trough sizes



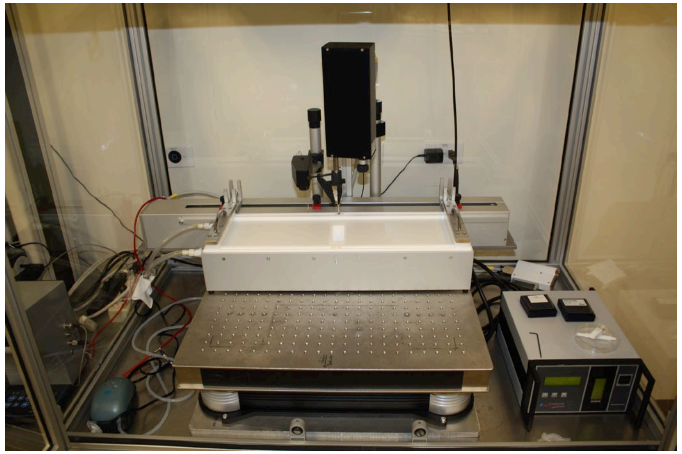
Trough	Surface Area (cm^2)	Subphase Volume (mL)	Compression Ratio
Extra Small	150	18	8.7
Small	98	57	5.2
Medium	273	176	10.8



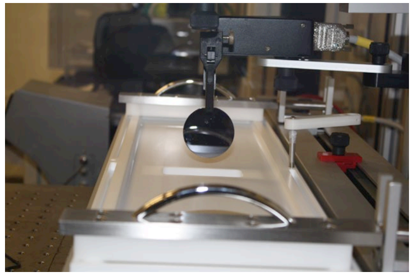
- Hermetically sealed enclosure
  - Sapphire windows for beam transport
  - Large viewing area
- Active vibration isolation

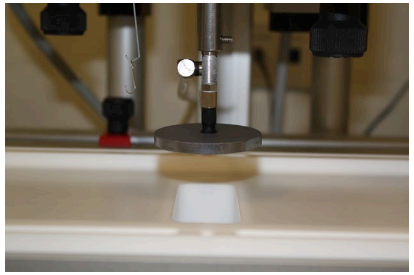
[Galuska L., Muckley E.S., Cao Z., Ehlenberg D., Qian Z., Zhang S., Rondeau-Gagne S., Phan M.D., Ankner J.F., Ivanov I., Gu X., "SMART transfer method to directly compare the mechanical response of water-supported and free-standing ultrathin polymeric films", Nature Communications 12, 2347 (2021)]

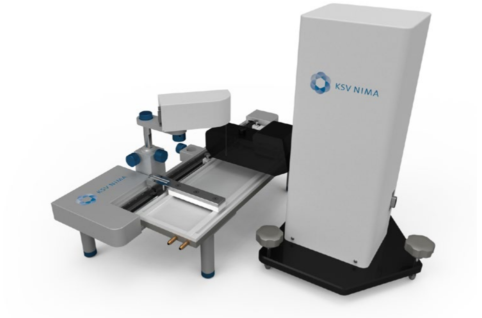
Langmuir film deposition



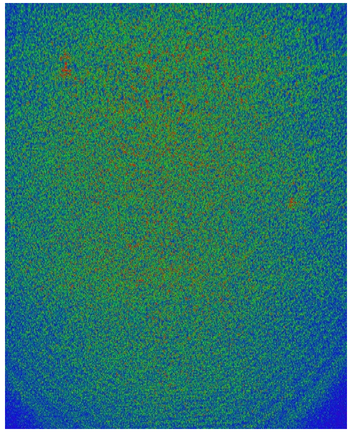
- KSV 2000 Dual-Barrier Trough
  - Large dipping well: 100 x 100 x 35 mm^3
  - Subphase temperature control
  - Total subphase volume: 1.2 L
  - Active vibration isolation







- KSV NIMA micro BAM
  - Fixed angle-of-incidence – 53^{o}
  - Large fields of view – 3600μm x 4000μm
  - 12 μm resolution
  - Still images as well as real-time video



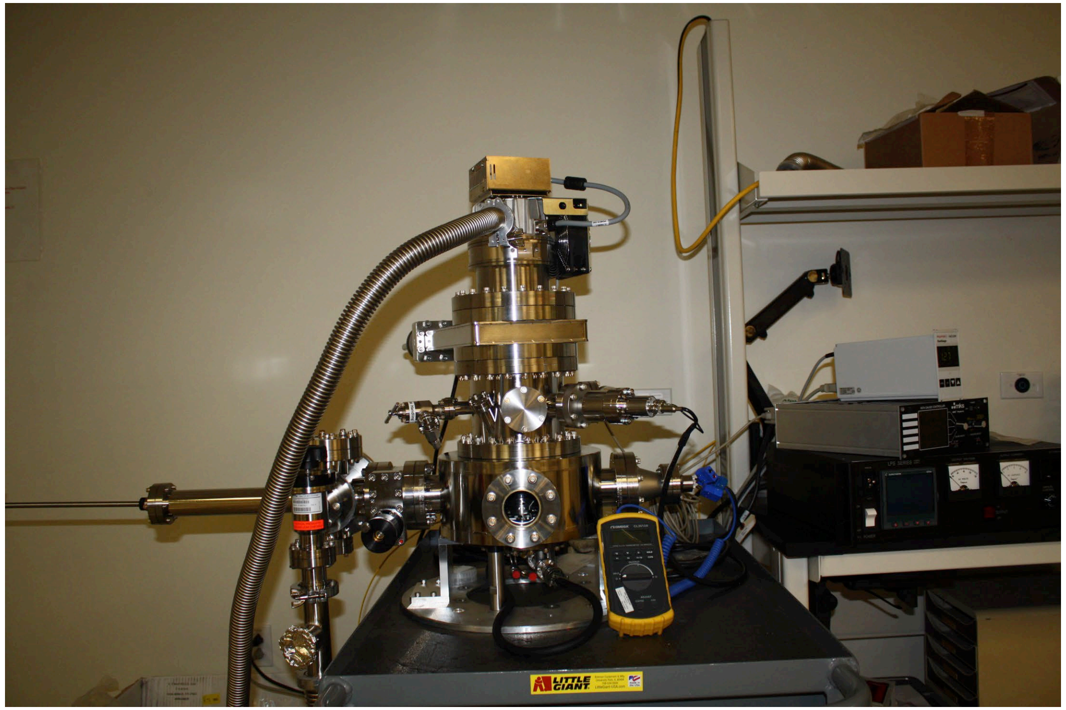
μ-BAM image of P3HT-b-PEOT on water subphase

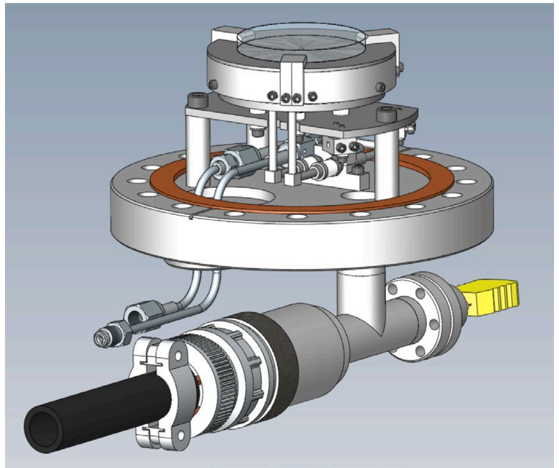
- KSV NIMA Surface Potential Meter (SPOT)
  - $\mu_n = \Delta V \cdot \varepsilon \cdot \varepsilon_0 \cdot A$
  - Determine effective dipole moment
  - Determine molecular orientation
  - Monitor complex formation between monolayers, subphase species and adsorbates

Rheology

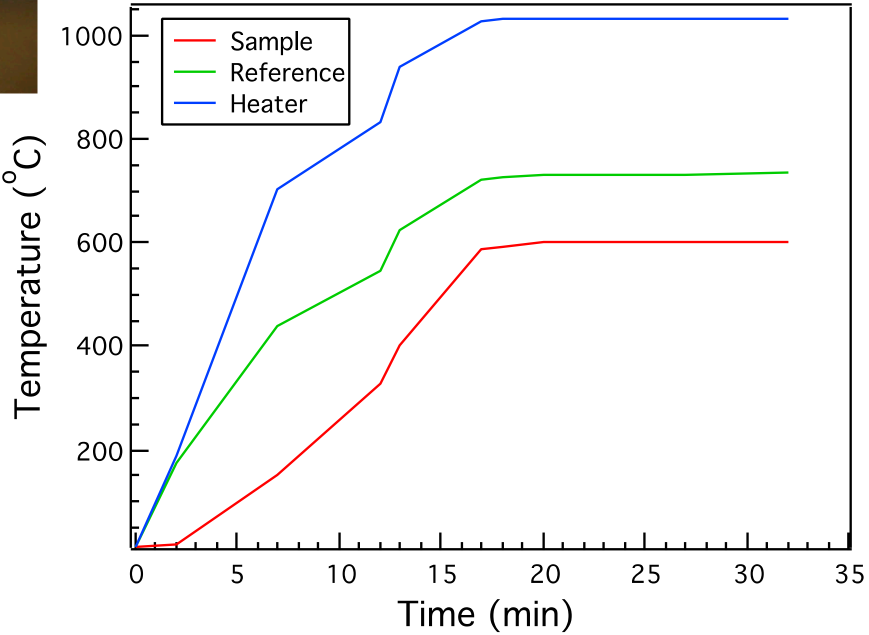
- Anton Paar MCR 501
  - Measuring geometries
    - Cone-plate (Ti cone w/ single crystal Si base plate)
    - Plate-plate (Ti plate w/ single crystal Si base plate)
    - Cup and bob (quartz for RheoSANS and quartz and Al for bench top measurements)
  - Temperature control
    - Convection (-50 ^{o}C to 200 ^{o}C)
    - Peltier (15 ^{o}C to 80 ^{o}C)
  - RheoSANS
    - Bin Wu from BSMD is actively developing a focus area in *in situ* rheological measurements in SANS
      - GP-SANS (HFIR) and EQ-SANS (SNS)

Multi-Environment Chamber



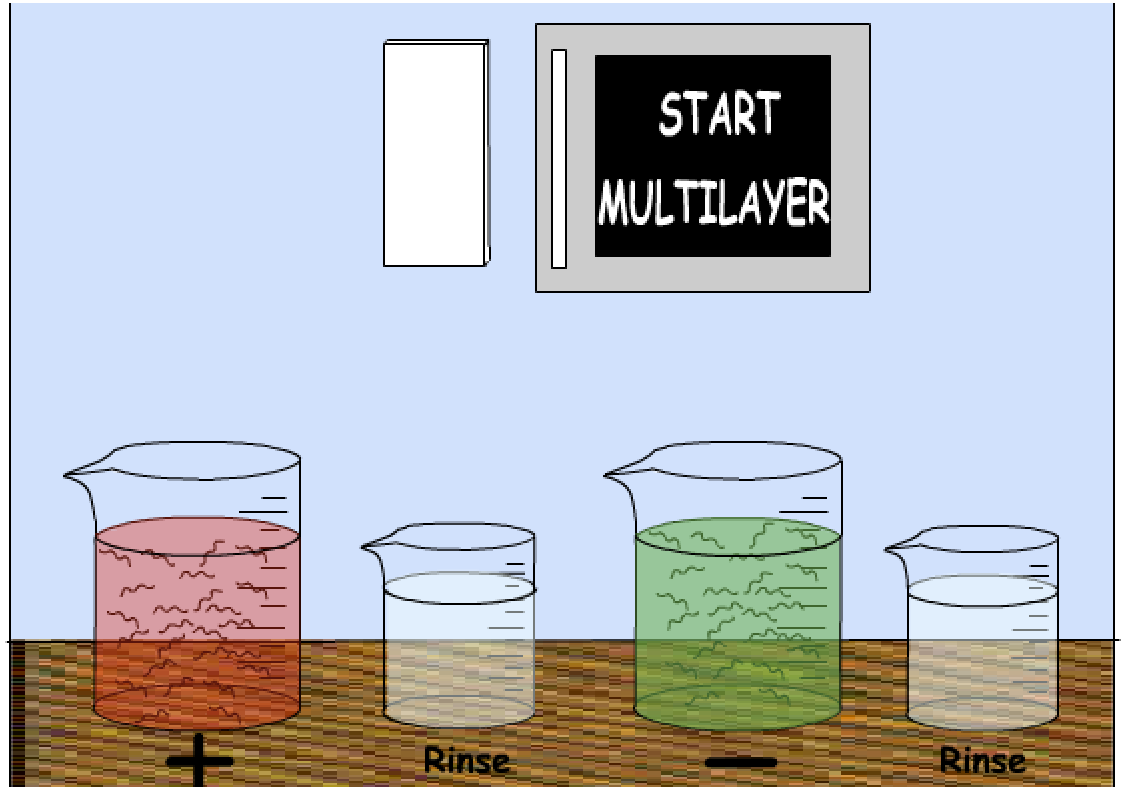


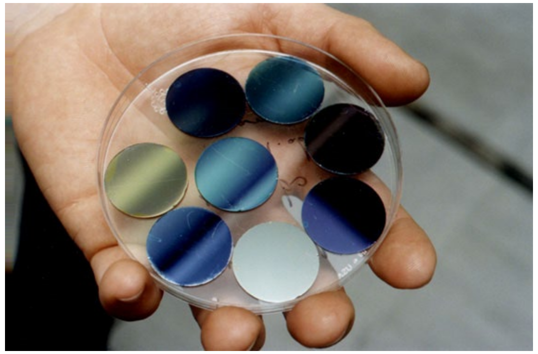
- Radiant resistive heater
  - Sample temperatures to 600 ^{o}C



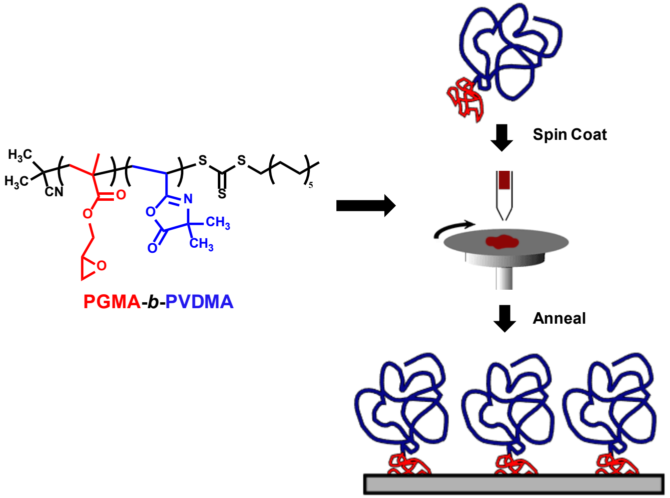
- Chamber base pressure ≤ 10^{-9} Torr
- For surface adsorption studies, *absolute* gas pressures in the range 0.001 Torr to 1000 Torr.

Layer-by-Layer (LbL) growth





- Simple
- Versatile – vast inventory of polyelectrolytes
- Environmentally friendly – aqueous, room temperature
- No limitation on substrate shape or size


PGMA-b-PVDMA
Spin Coat
Anneal