Defining QIKR

John F. Ankner

QIKR Instrument Scientist

QIKR Motion Preliminary Design Review

November 6, 2024

Oak Ridge National Laboratory

Defining QIKR

1. Big picture
2. Required Q range
3. Measure in a single setting
4. Bring source to sample
5. Enable *θ*-*θ* geometry
6. Required resolution
7. Beam definition at sample
8. Positioning the detector
9. Summary – put it together

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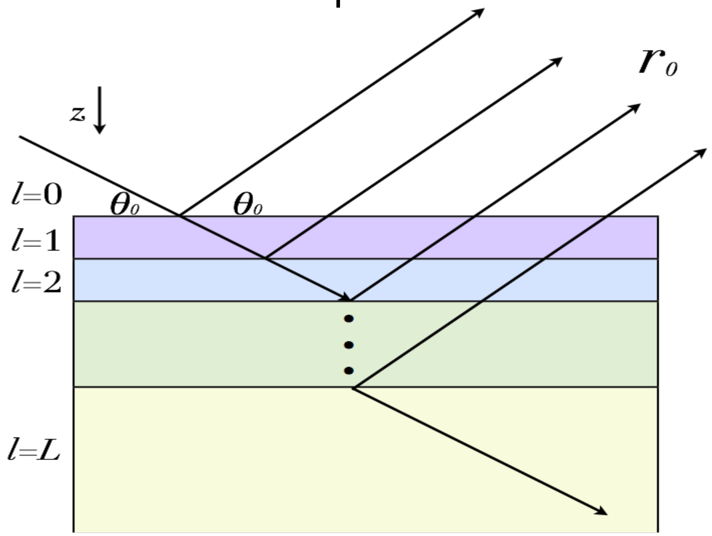
QIKR will make time-resolved reflectometry routine

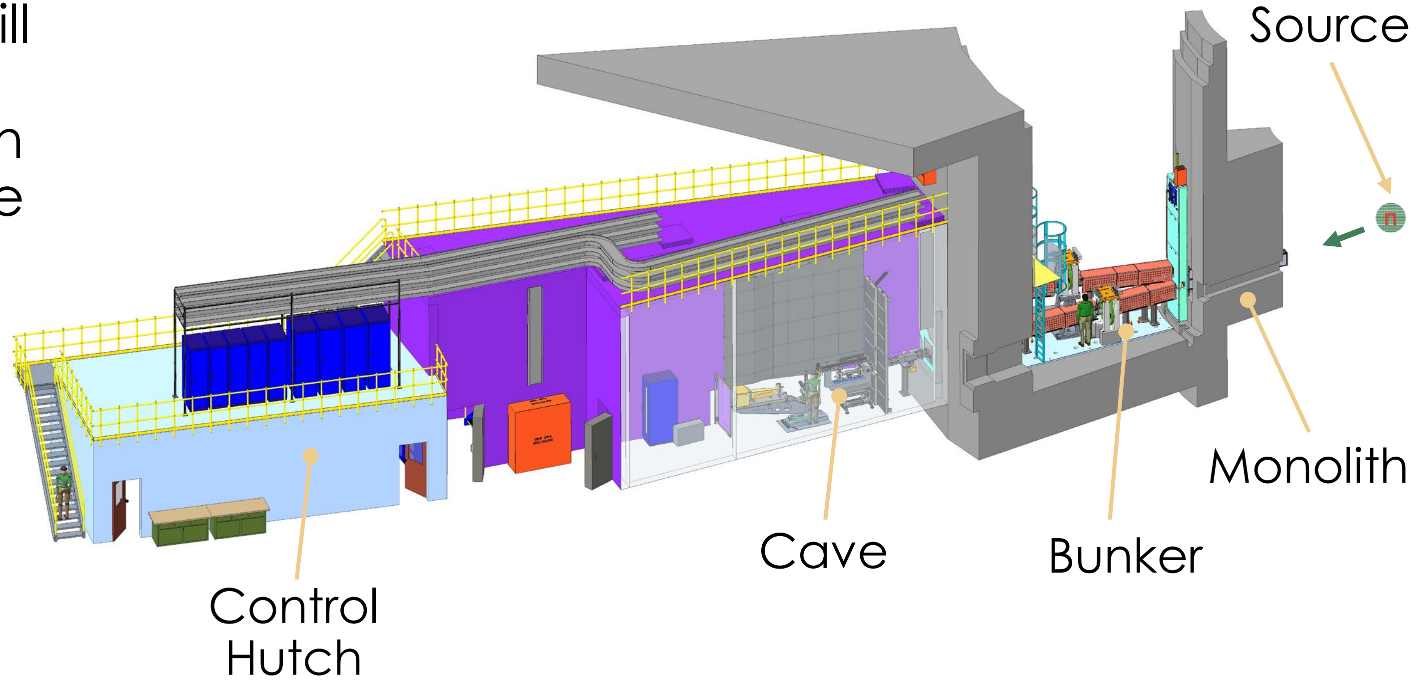
STS flux and wavelength bandwidth will enable routine single-setting measurement of specular reflectivity in seconds to minutes, depending on the sample



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

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

[Density × Avogadro's number / Molecular mass]

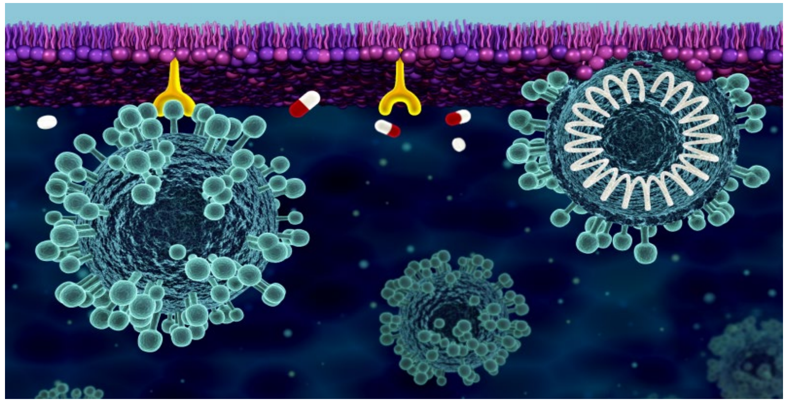


"Cinematic" data collection at one instrument setting and event-based data reduction will enable post-experiment tracking of structural evolution in time over a broad scientific landscape

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

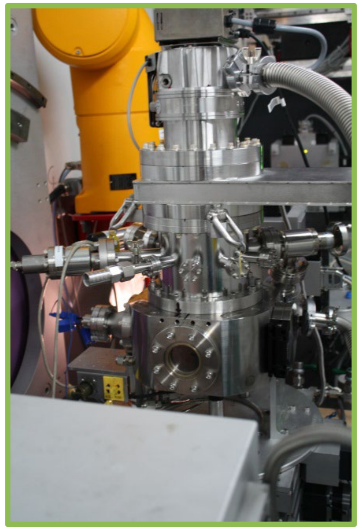
Energy Materials
- Solid-electrolyte interphase
- Organic photovoltaics
- Ionic liquids
- Corrosion
- Mesoporous films
- Conjugated polymer films
- Metal-harvesting polymers

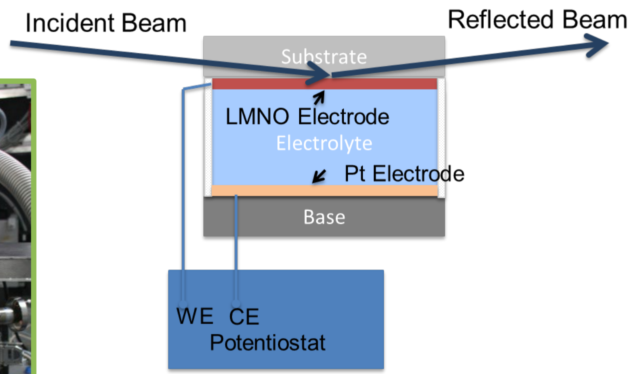


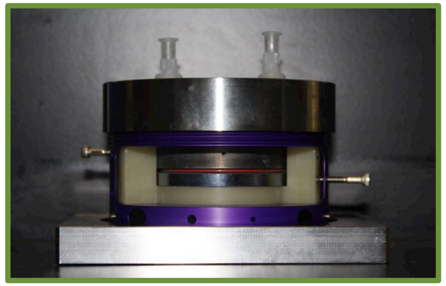
[Courtesy R. Ashkar]

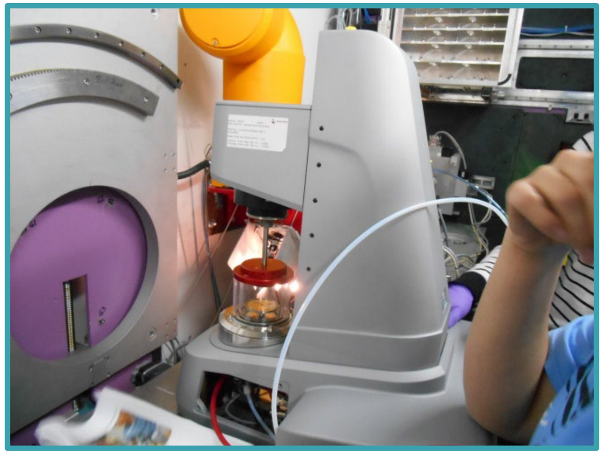
Biomaterials
- Model membranes
- Lipid flip-flop
- Structure of transmembrane peptides
- Biocompatible coatings
- Surfactant and phospholipid monolayers
- Drug delivery
- Protein conformation to membranes
- Influence of synthetic nanoparticles on membrane structure

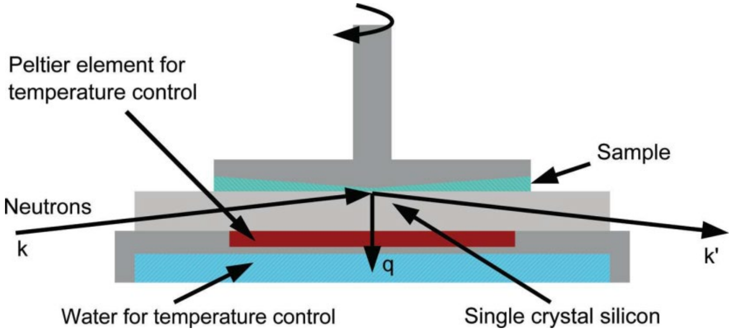
Diverse environments



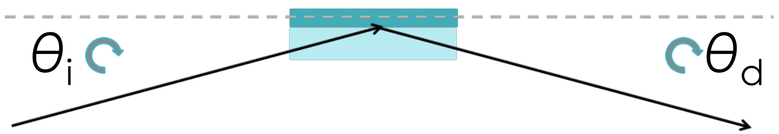






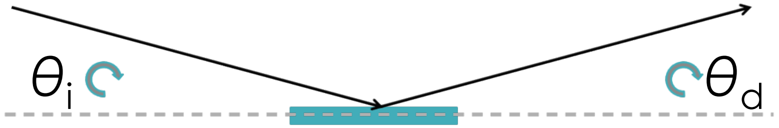


$\theta_s = 0$, fixed



θ-θ geometry

$\theta_d = -\theta_i$

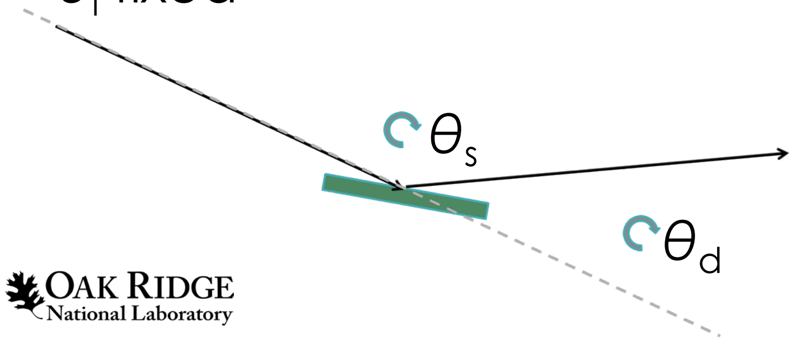


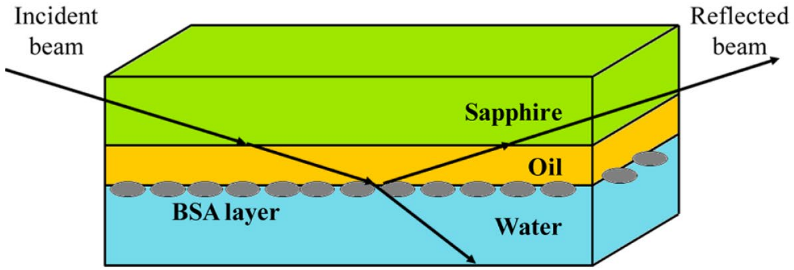
$\theta_s = 0$, fixed

θ-2θ geometry

$\theta_d = 2\theta_s$

θ_i fixed





Two end stations

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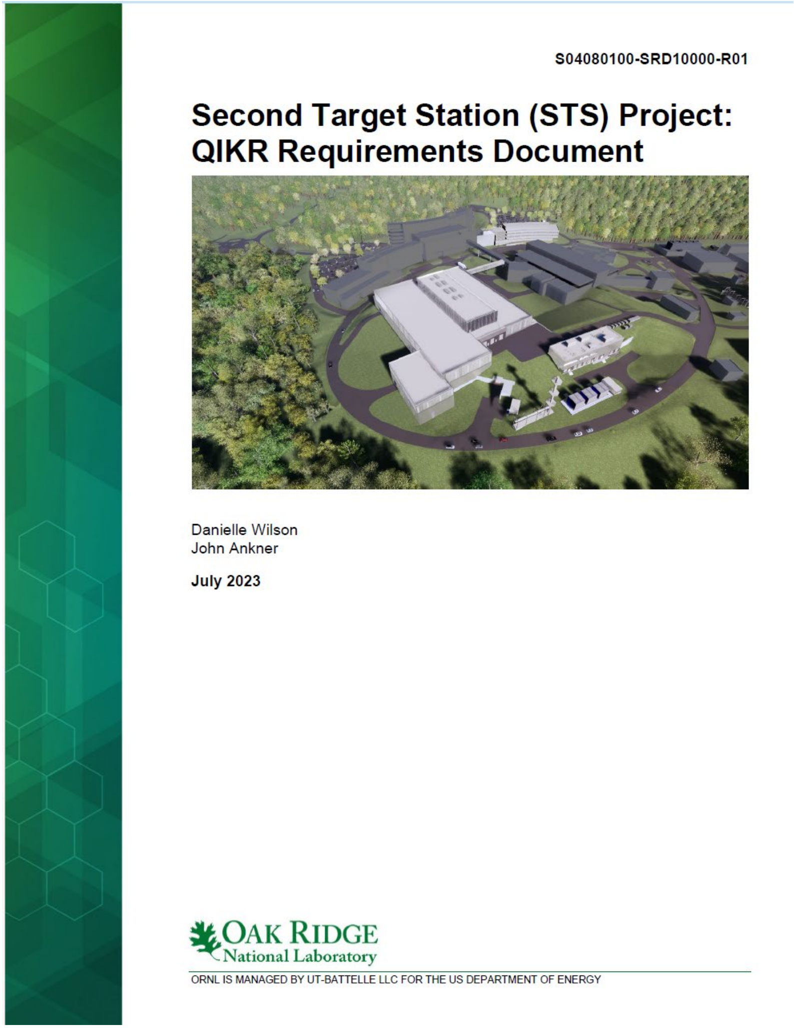
QIKR requirements

Entire Instrument


S04080100-SRD10000-R01

Second Target Station (STS) Project: QIKR Requirements Document

Danielle Wilson
John Ankner

July 2023

OAK RIDGE National Laboratory

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Motion


S04080600-SRD10000-R00

Second Target Station Project:

QIKR Motion Systems Requirements Document

Rudolf Thermer
Danielle Wilson

October 2024

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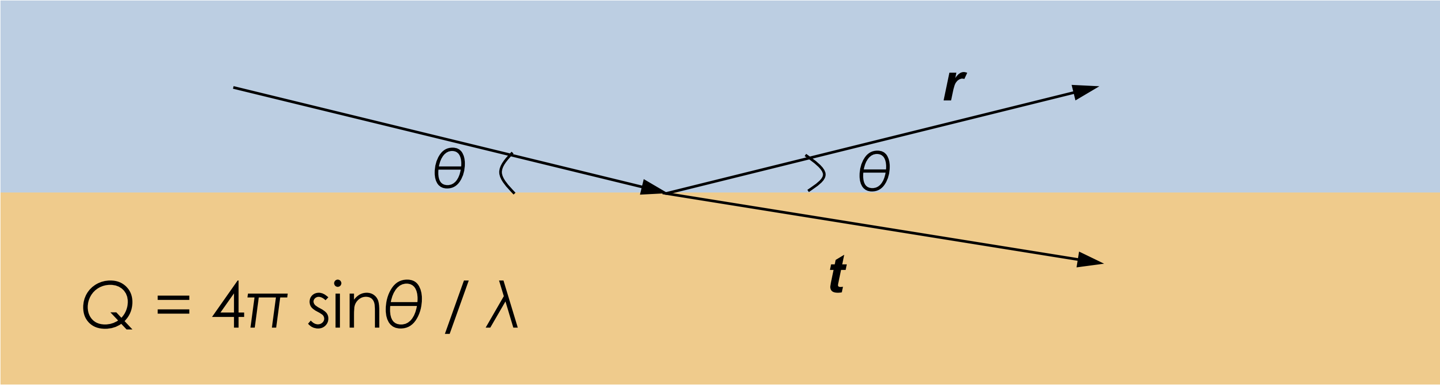
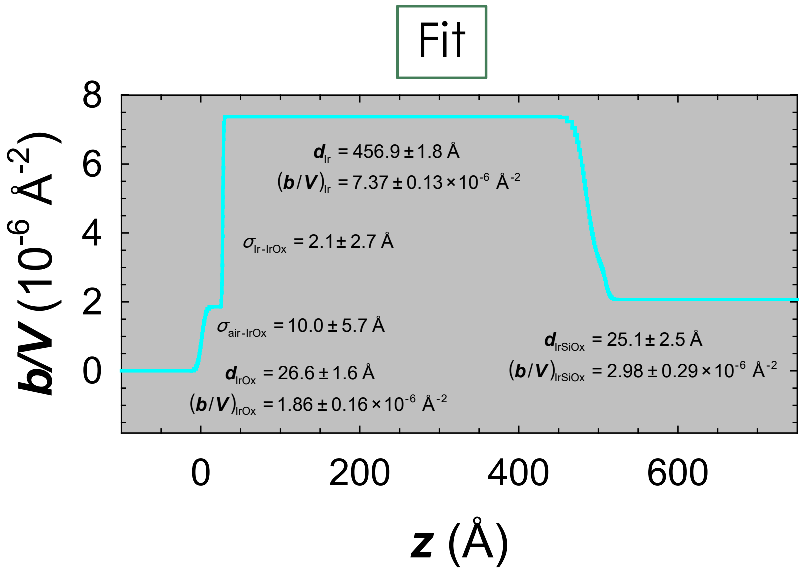
Neutron reflectivity from Ir/Si standard



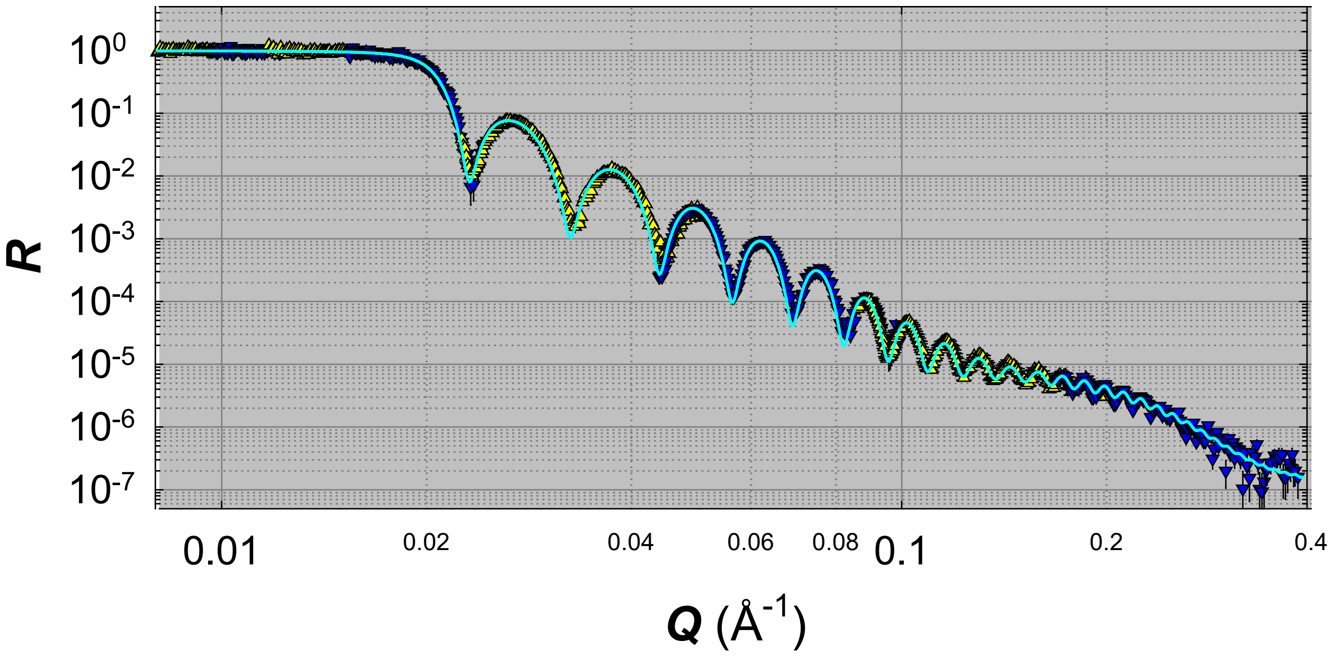


NR characterized by wavevector Q, a function of incident angle θ and wavelength λ

- No useful information below Q_{min}
- Q_{max} background limited

=> $0.005\ Å^{-1} < Q < 0.5\ Å^{-1}$

[Req. S.04.08.02-R3]



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Single setting Q range

Wavevector transfer

$$Q = 4\pi \sin\theta / \lambda$$

and wave-particle duality

$$h^2 / 2m\lambda^2 = mv^2 / 2$$

determine Q dynamic range

$$\frac{Q_{\max}}{Q_{\min}} = \frac{\lambda_{\max}}{\lambda_{\min}} = 1 + \frac{h}{m}\frac{1}{L}\frac{1}{f}\frac{1}{\lambda_{\min}} \equiv D$$

where

h/m = 3956.0 m-Hz-Å

L = instrument length (m)

f = repetition rate (Hz)

λ_{min} = minimum wavelength (Å)

[Reqs. S.04.08.01-R21;-R22;-R24]

STS QIKR-L

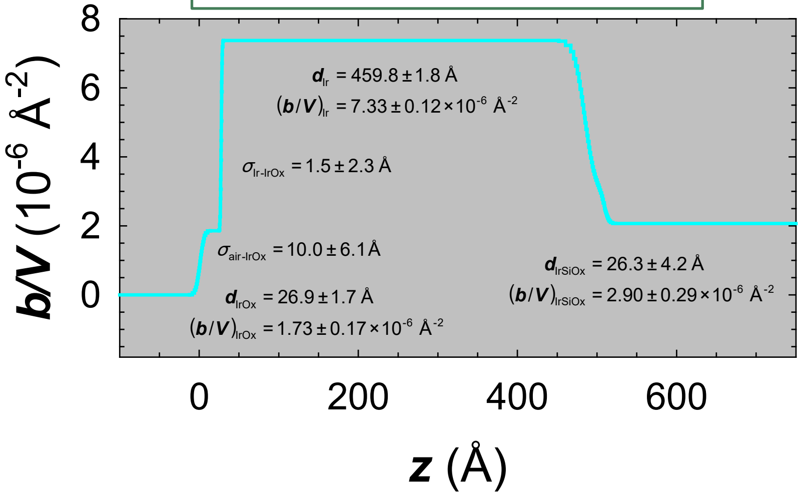
L = 20.0 m

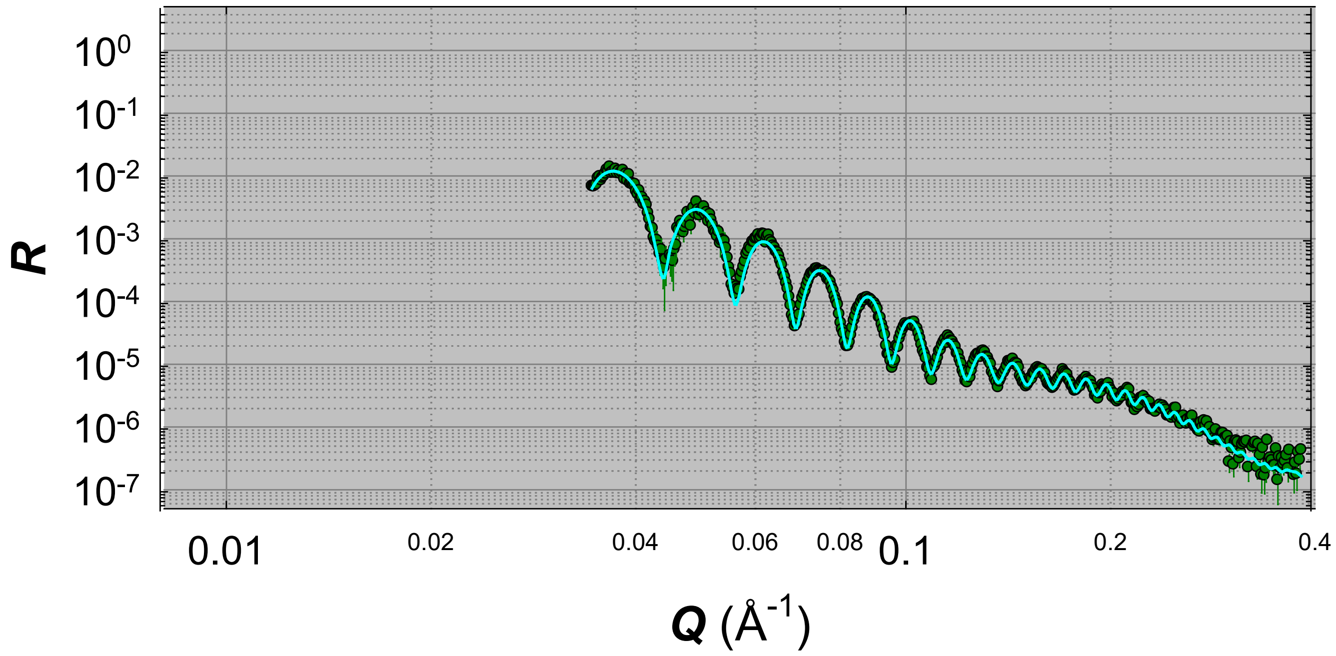
f = 7.5 Hz

λ_{min} = 2.5 Å

D = 11.5

Equivalent fit quality to full Q range





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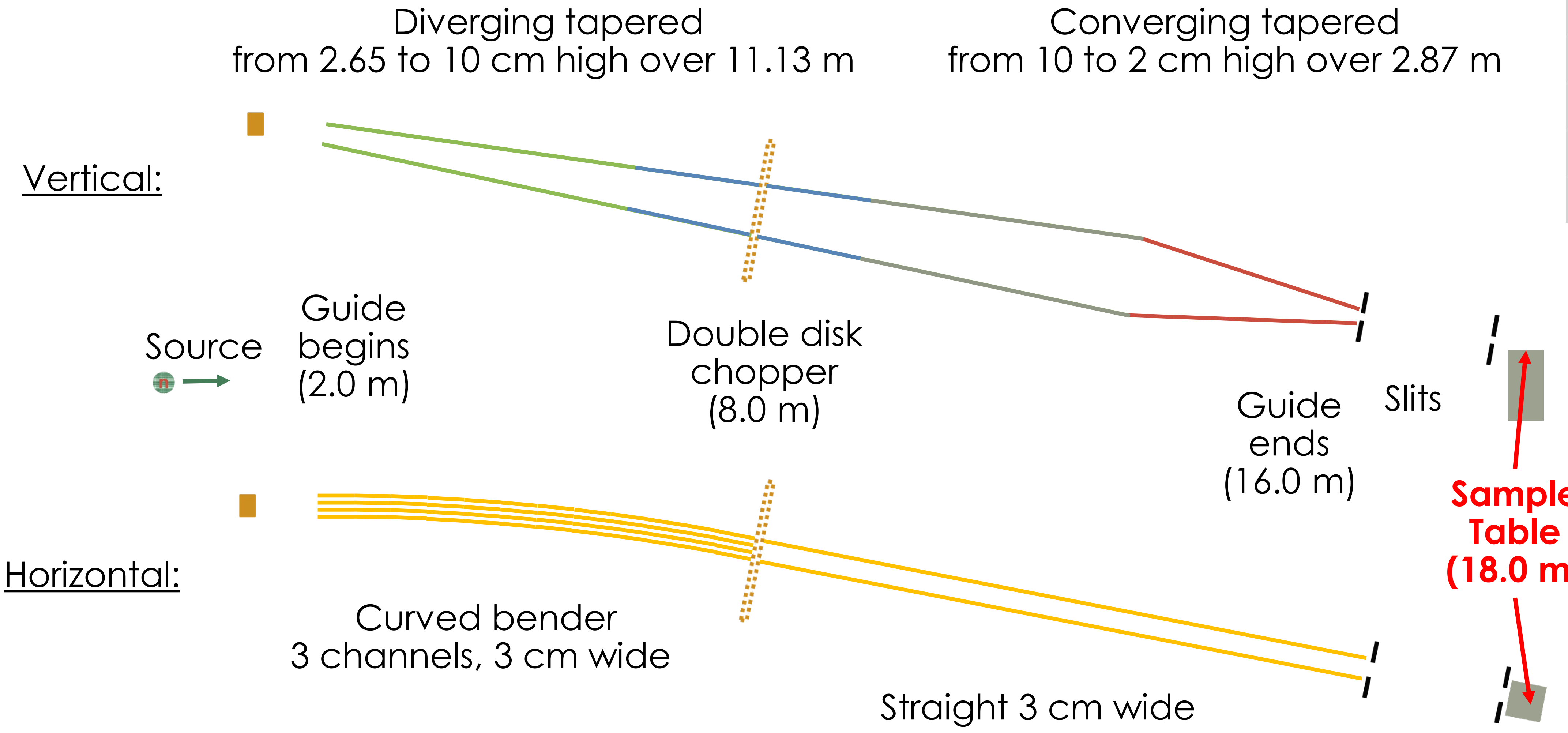
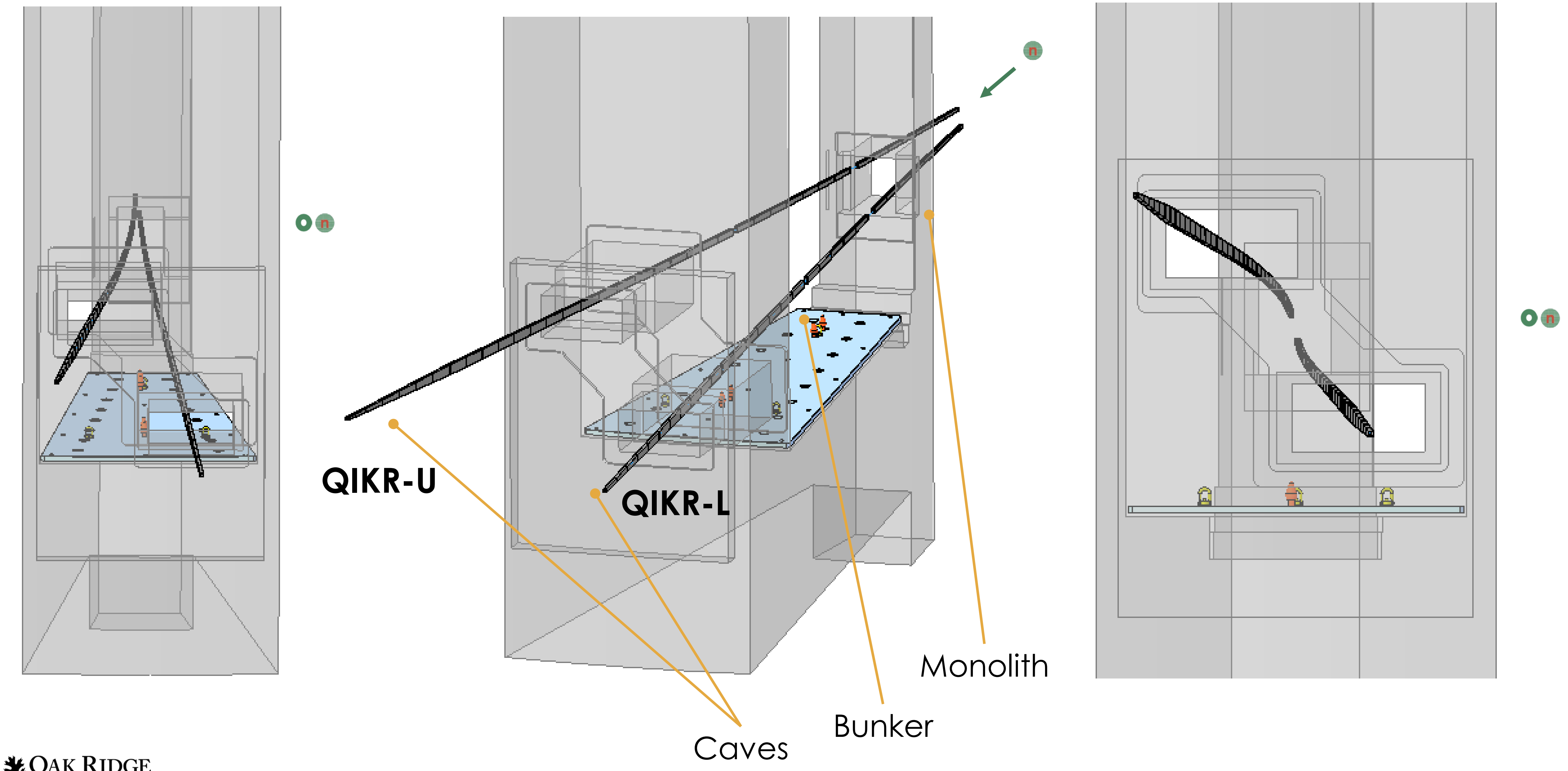
Transport source to sample (QIKR-L)



Guide *m*	
0	gray
1	blue
2	green
3	yellow
4.5	red

Neutron guide filters out unwanted neutrons, delivering wanted neutrons (3×2 cm^2) to the sample
[Reqs. S.04.08.01-R21;-R23;-R24;-R25]

Guide views – looking upstream



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Operate in θ-2θ and θ-θ geometries

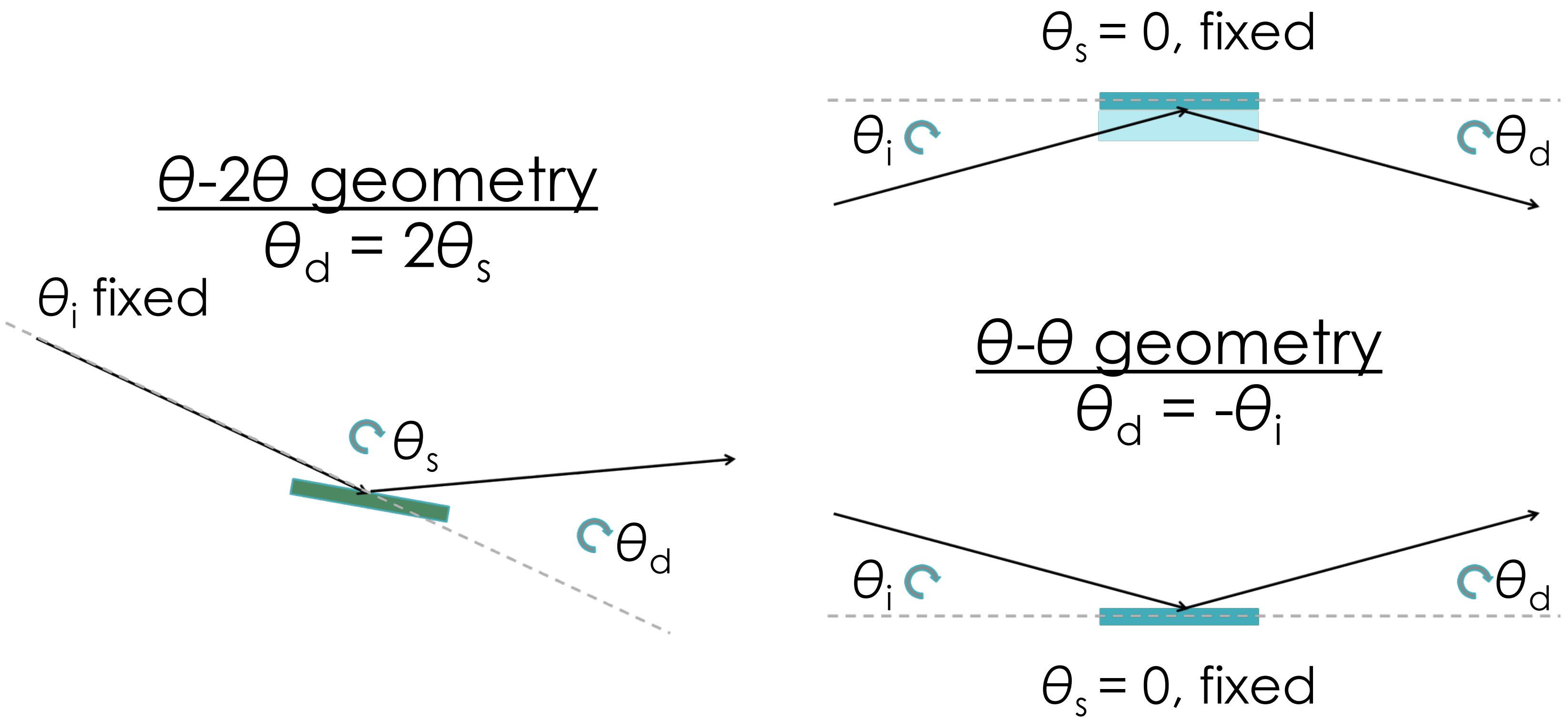
θ-2θ geometry

- Incident beam fixed
- Sample moves
- Detector moves

θ-θ geometry

- Incident beam varies
- Sample fixed
- Detector fixed

[Reqs. S.04.08.01-R7;-R12]



Guide system provides multiple beams for θ-θ

<u>Characteristics</u>

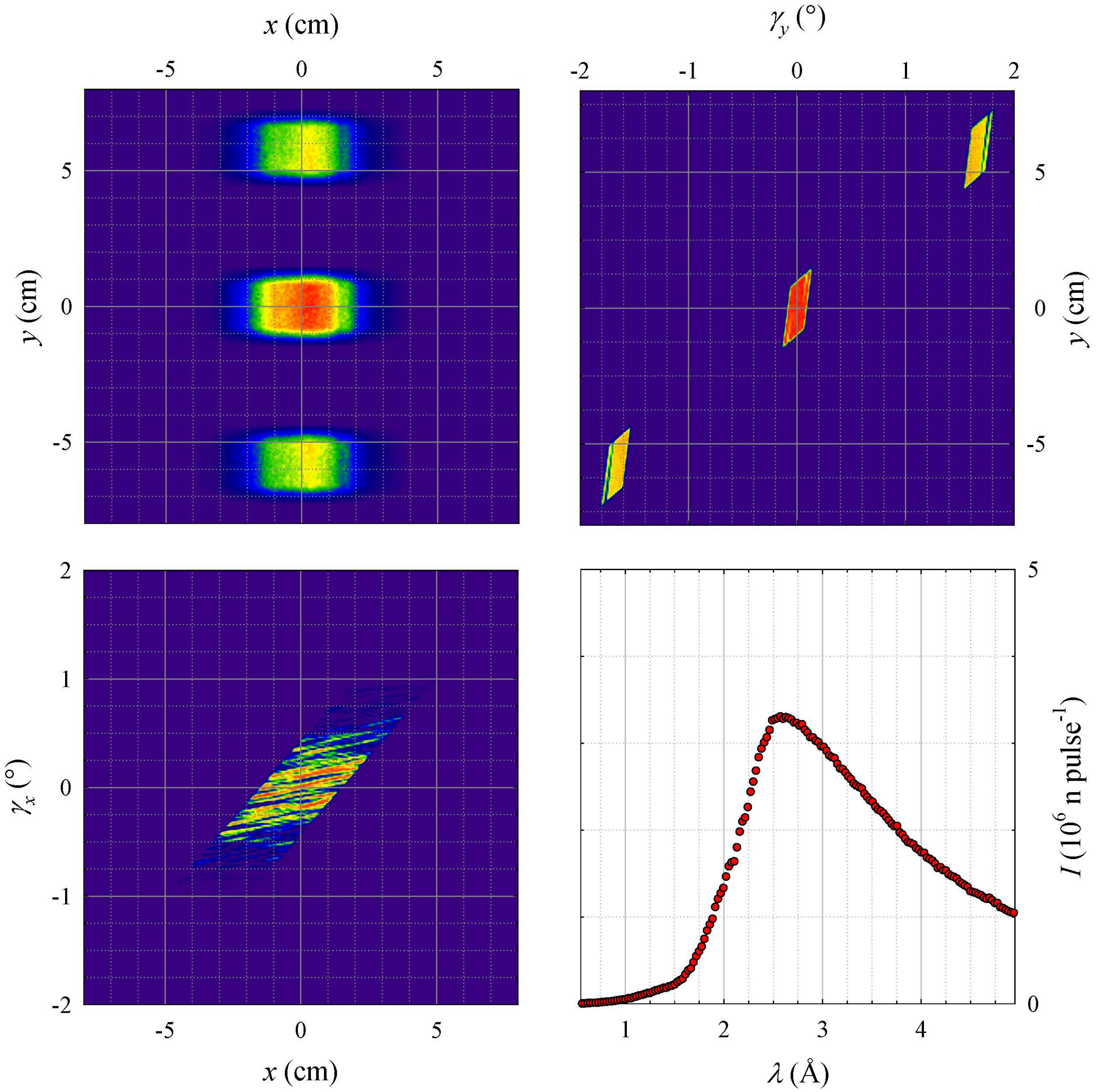
Three beams

…separated in space (y)

…and angle γ_y

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

[Reqs. S.04.08.01-R3;-R14]



(QIKR-L McStas simulation)

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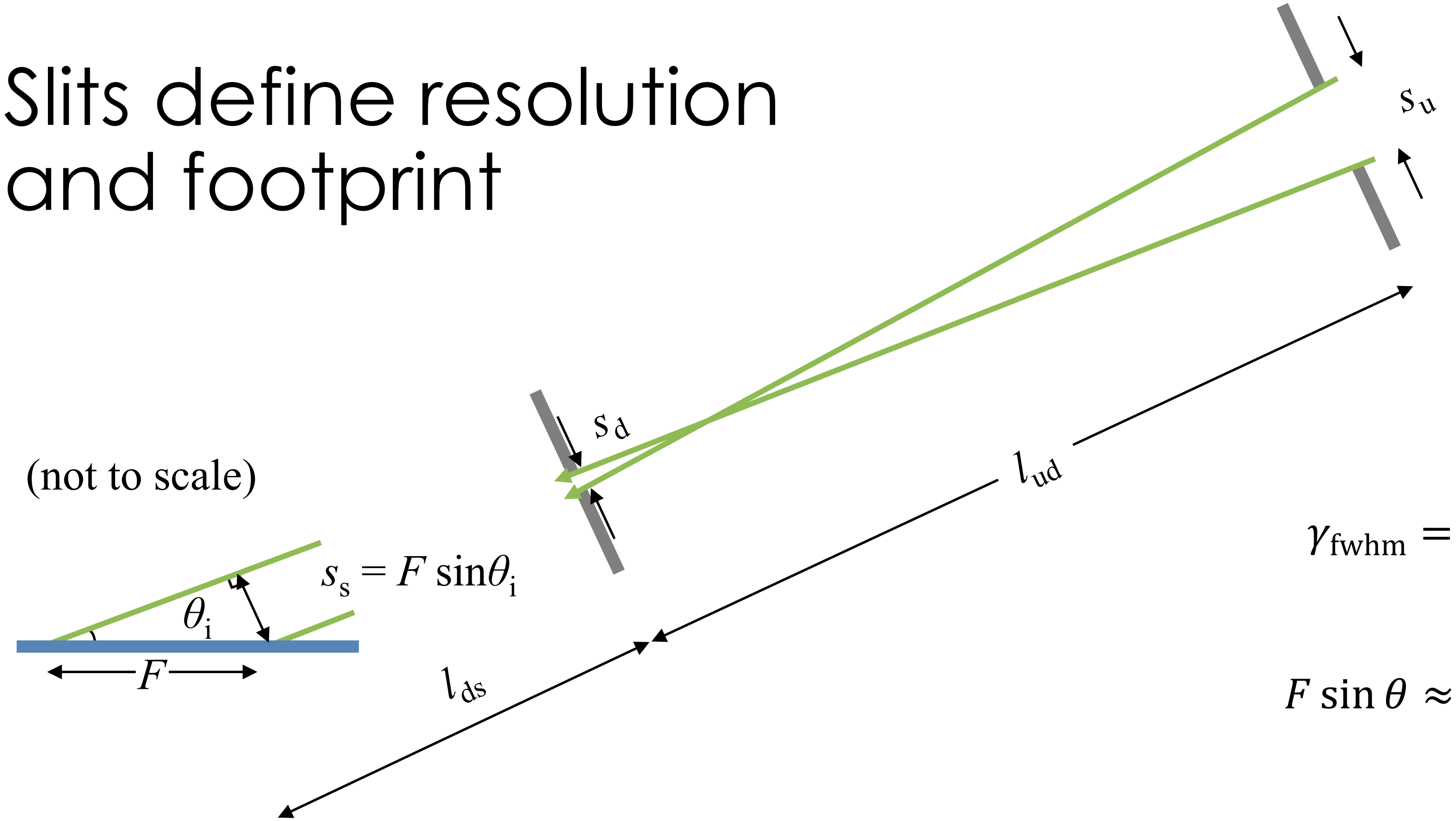
Slits define resolution and footprint



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

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

Which slit settings s_u and s_d will confine beam within footprint F at incident angle θ with angular divergence $(\delta\theta/\theta)$?

=>

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

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

What is the integrated acceptance?

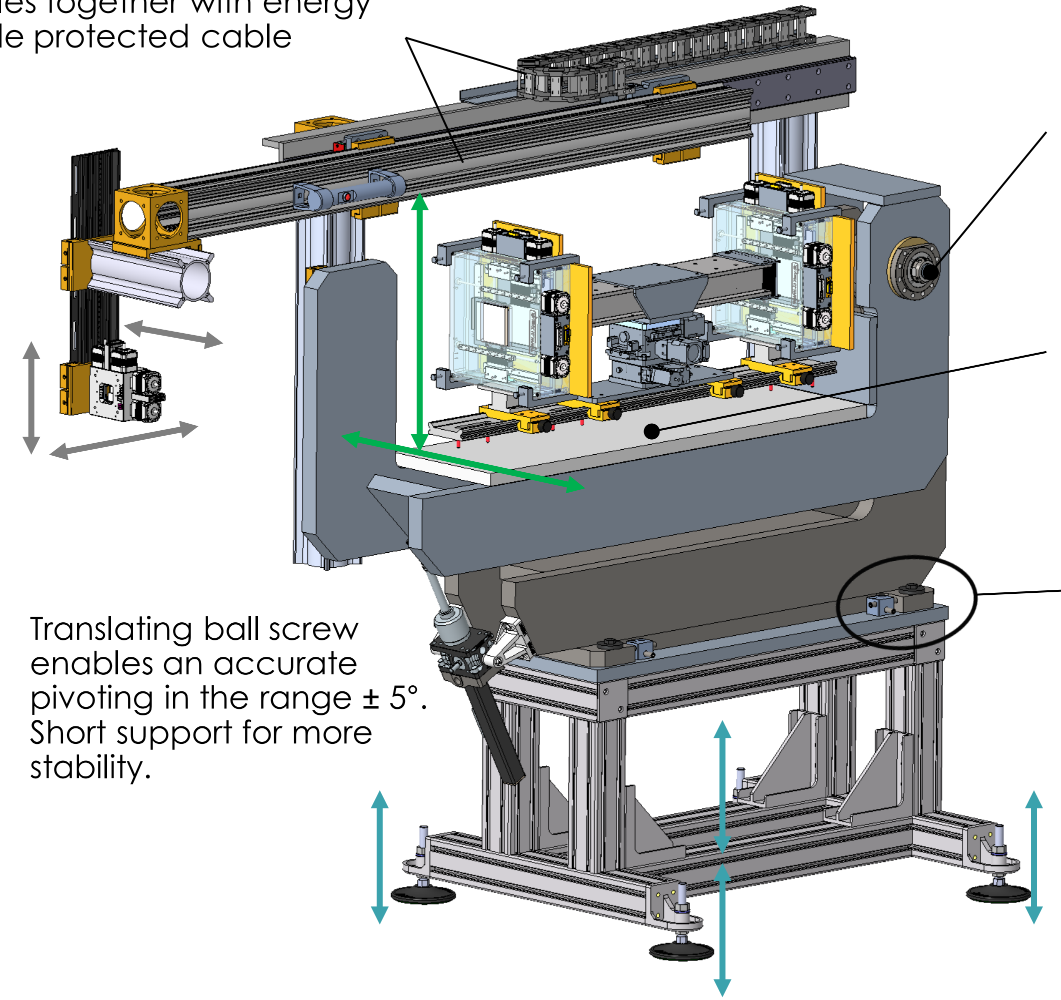
$$A = \frac{s_u s_d}{L_{ud}}$$

Incident Table – holds slits and optics

Preliminary design of an incident table for QIKR

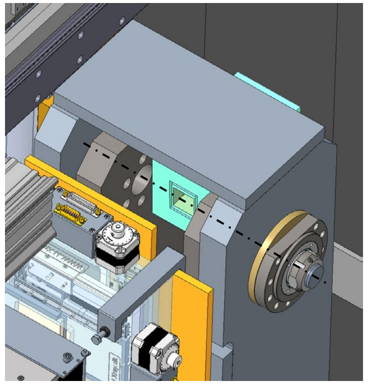
Hollow profiles together with energy chain enable protected cable installation.

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



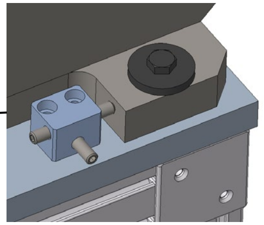
Translating ball screw enables an accurate pivoting in the range ± 5°. Short support for more stability.

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]

Footprint calculator – maximum slits

Resolution

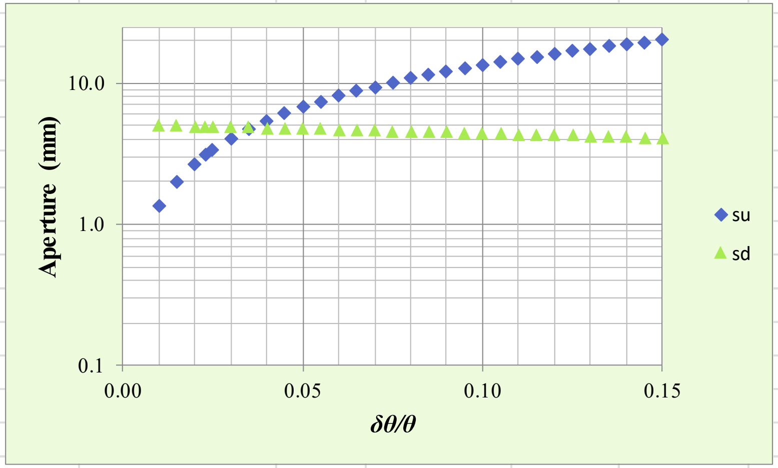
$0.02 < \delta\theta/\theta < 0.07$

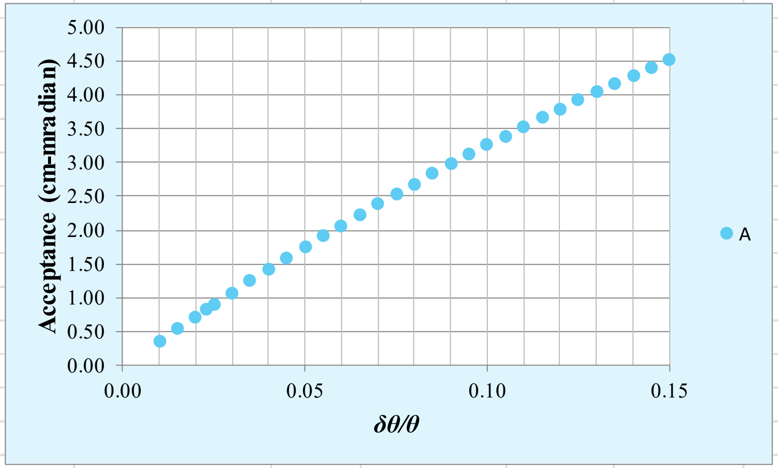
implies

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

[Reqs. S.04.08.06-R107; -R108;-R110;-R111;-R114]

	$\delta\theta/\theta$	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





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Footprint calculator – minimum slits

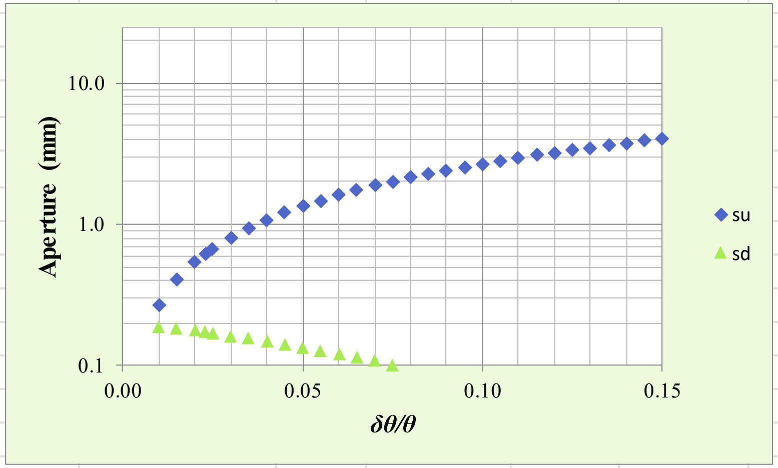
Beam Size and Footprint

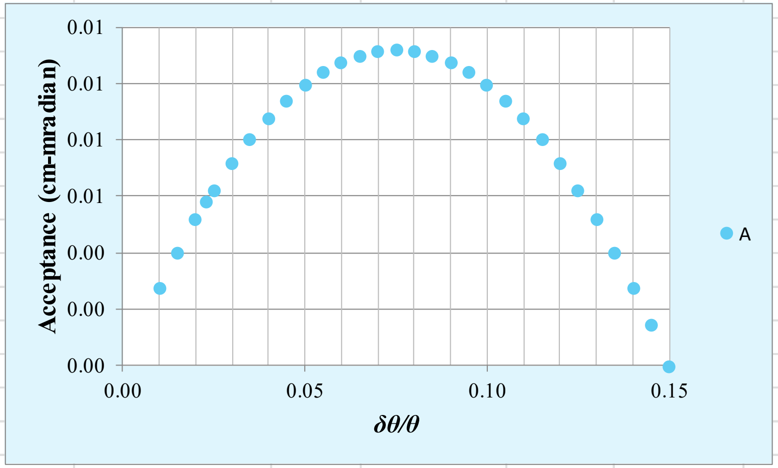
- Smallest: 0.1 mm
- $\delta\theta/\theta = 0.02$ @ $\theta = 0.5°$ => $\delta\theta = 0.01°$

[Reqs. S.04.08.06-R119; -R123]

θ (º)	0.83
L_{ud} (mm)	1875.0
L_{ds} (mm)	100.0
F (mm)	15.0

$\delta\theta/\theta$	s_u (mm)	s_d (mm)	A (cm-mradian)
0.010	0.27	0.19	0.003
0.015	0.41	0.19	0.004
0.020	0.54	0.18	0.005
0.023	0.62	0.17	0.006
0.025	0.68	0.17	0.006
0.030	0.81	0.17	0.007
0.035	0.95	0.16	0.008
0.040	1.09	0.15	0.009
0.045	1.22	0.14	0.009
0.050	1.36	0.14	0.010
0.055	1.49	0.13	0.010
0.060	1.63	0.12	0.011
0.065	1.77	0.12	0.011
0.070	1.90	0.11	0.011
0.075	2.04	0.10	0.011
0.080	2.17	0.10	0.011
0.085	2.31	0.09	0.011
0.090	2.44	0.08	0.011
0.095	2.58	0.08	0.010
0.100	2.72	0.07	0.010
0.105	2.85	0.06	0.009
0.110	2.99	0.06	0.009
0.115	3.12	0.05	0.008
0.120	3.26	0.04	0.007
0.125	3.40	0.03	0.006
0.130	3.53	0.03	0.005
0.135	3.67	0.02	0.004
0.140	3.80	0.01	0.003
0.145	3.94	0.01	0.001
0.150	4.07	0.00	0.000





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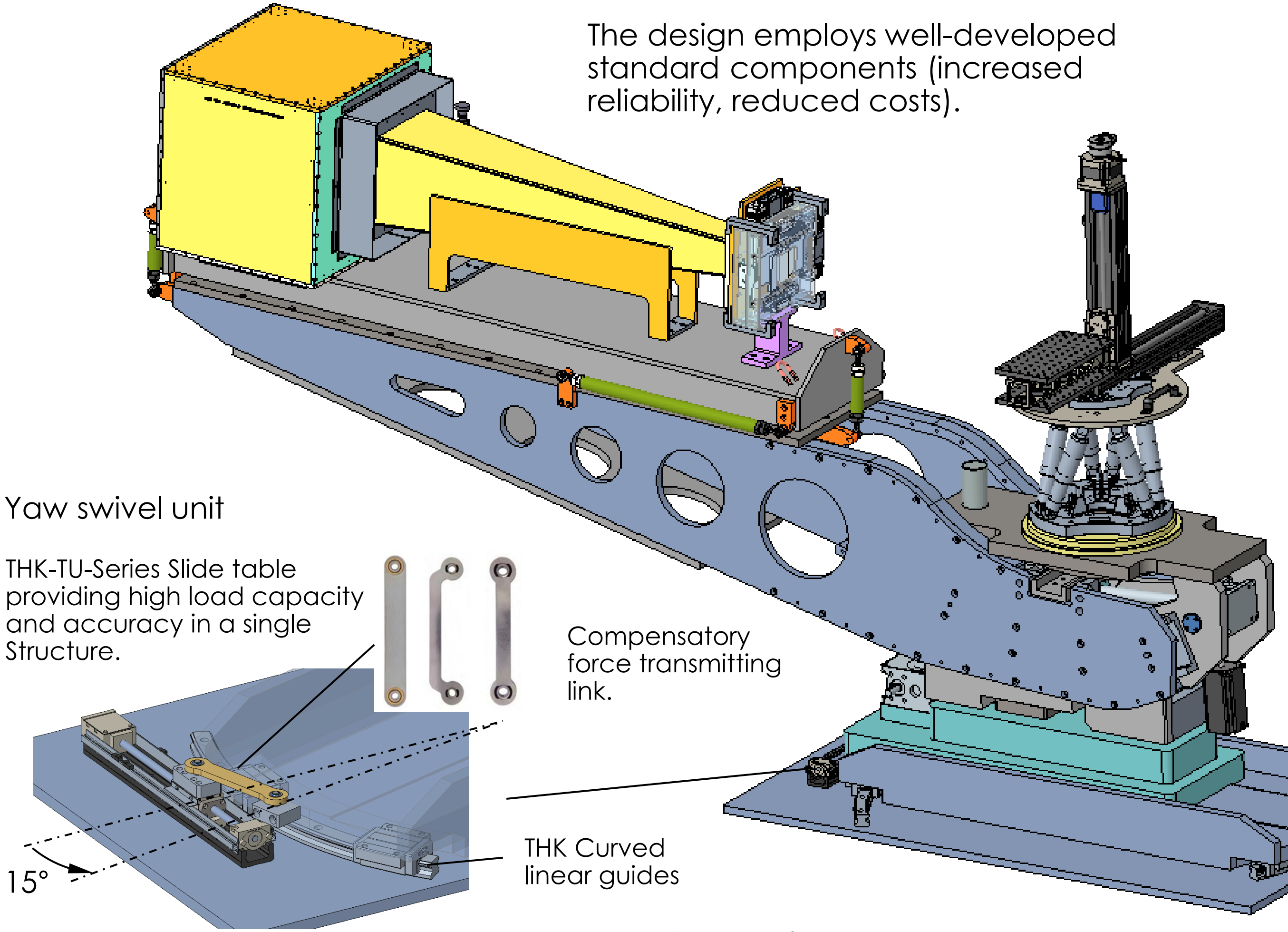
Sample Table and Detector Arm unit

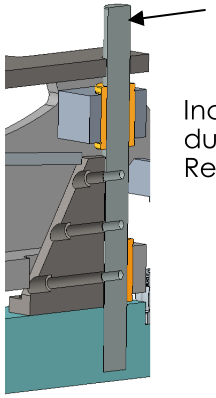
The design employs well-developed standard components (increased reliability, reduced costs).



PI H-850 Hexapod
Payload: 250 kg

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

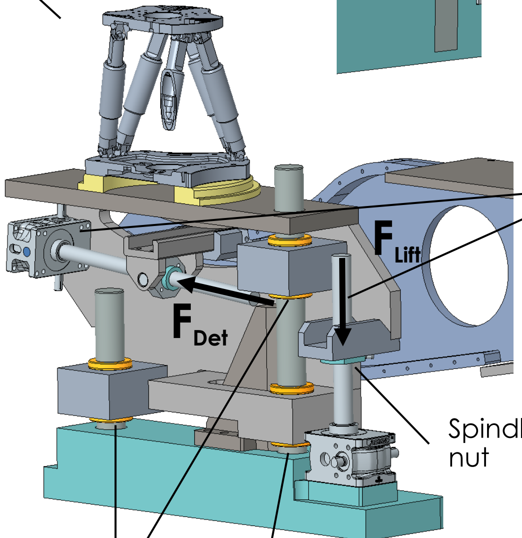
Robust guide system



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

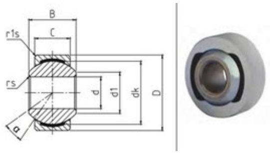
Yaw swivel unit

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!



Preloaded linear ball bushings

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

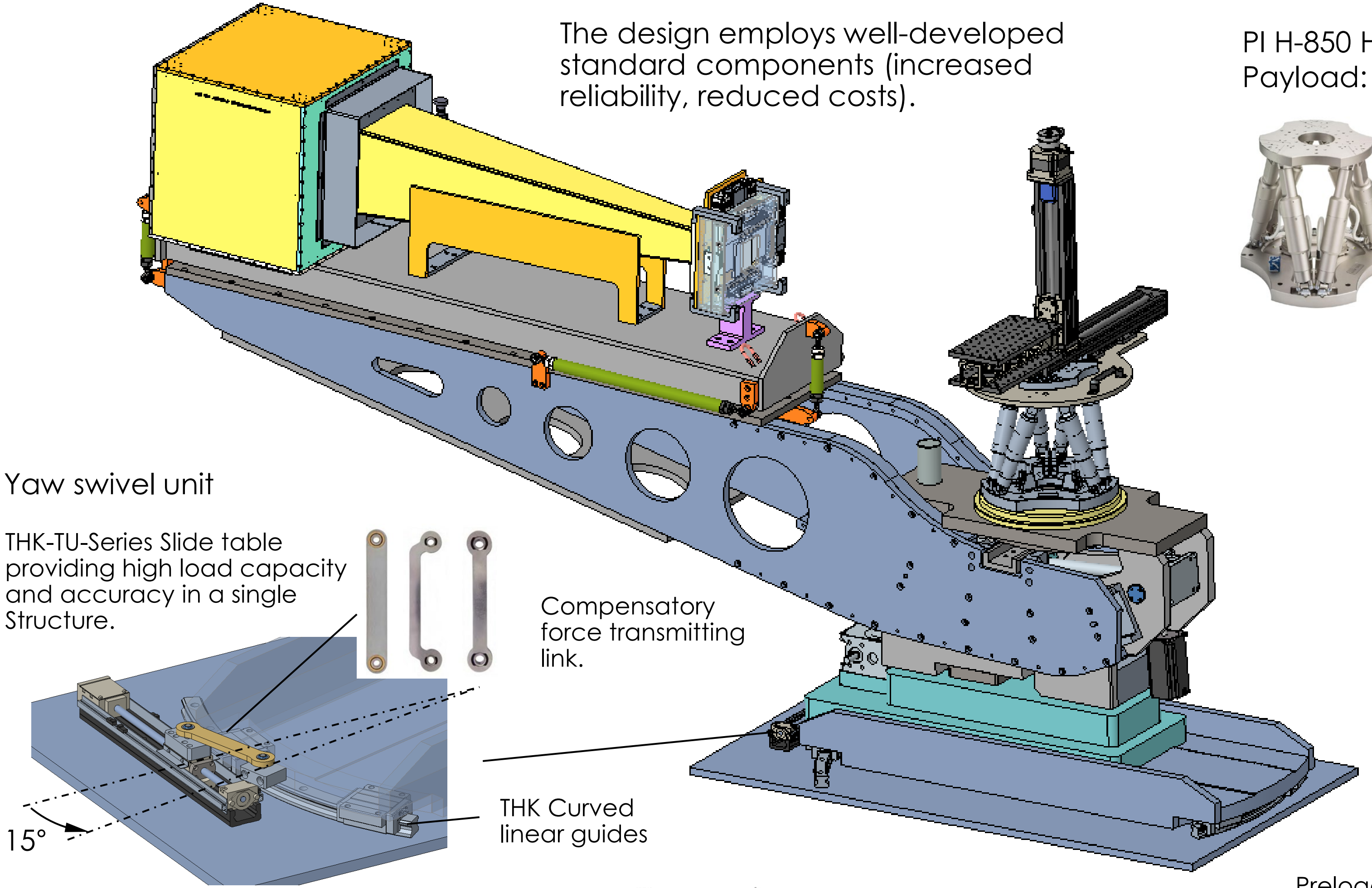
[courtesy Rudy Thermer]

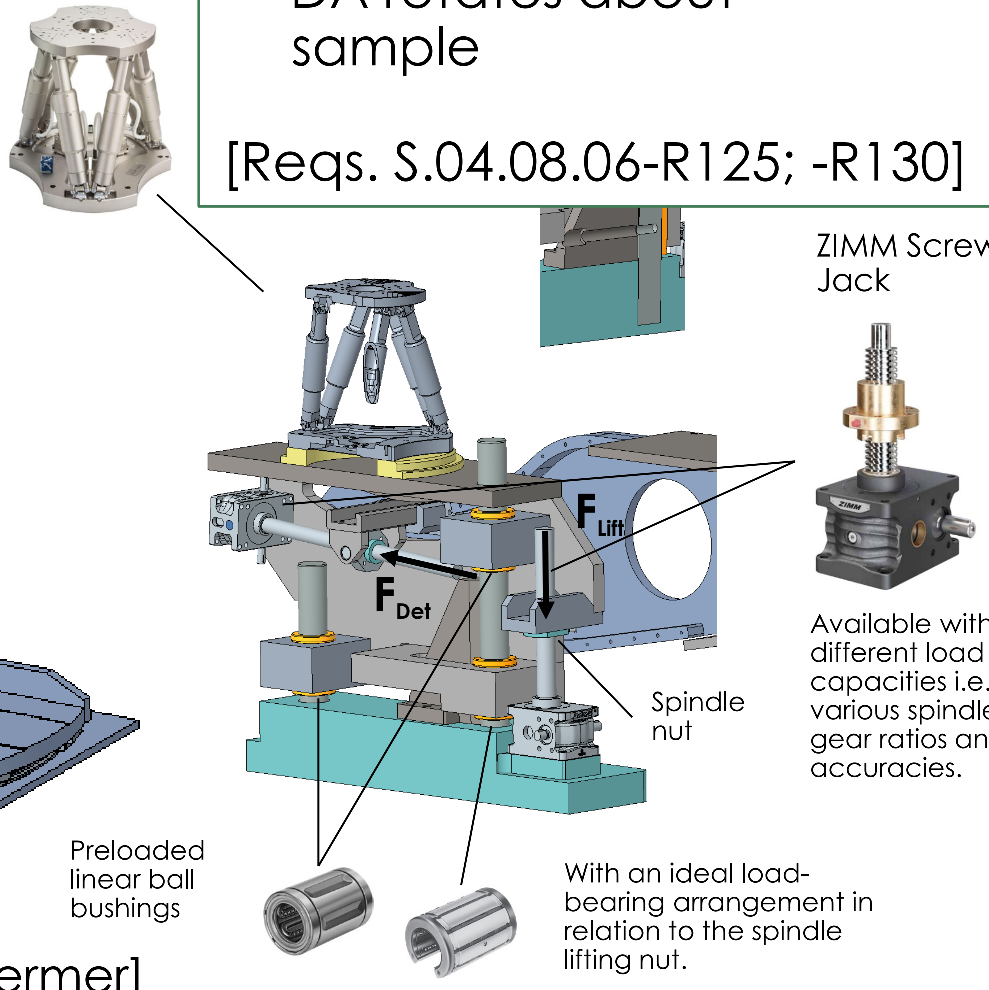
Sample Table and Detector Arm unit

Positioning

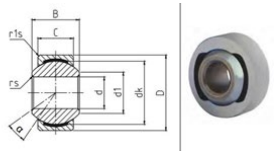
- Axes of ST and DA must coincide in beam
- DA rotates about sample

[Reqs. S.04.08.06-R125; -R130]





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



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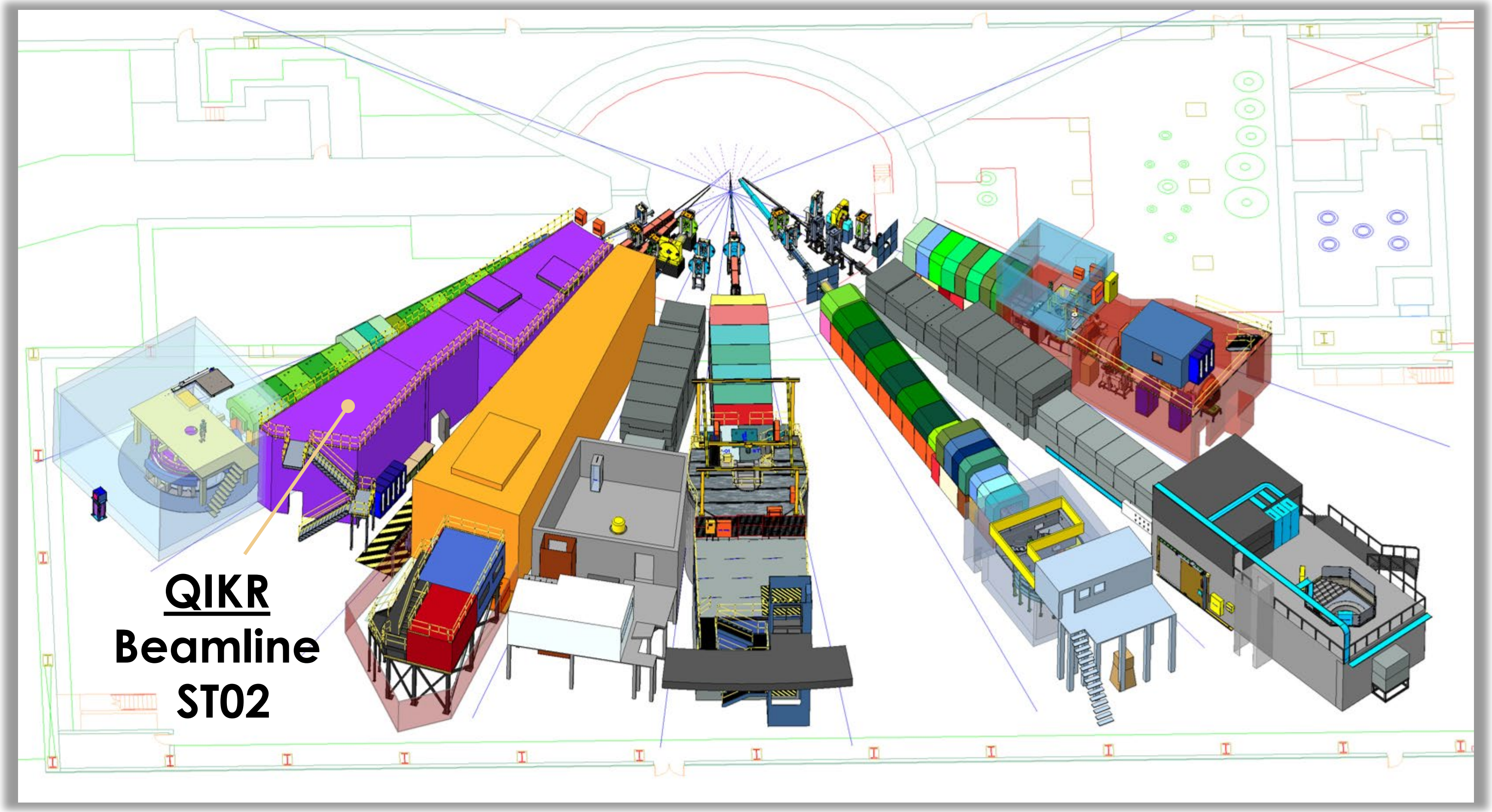
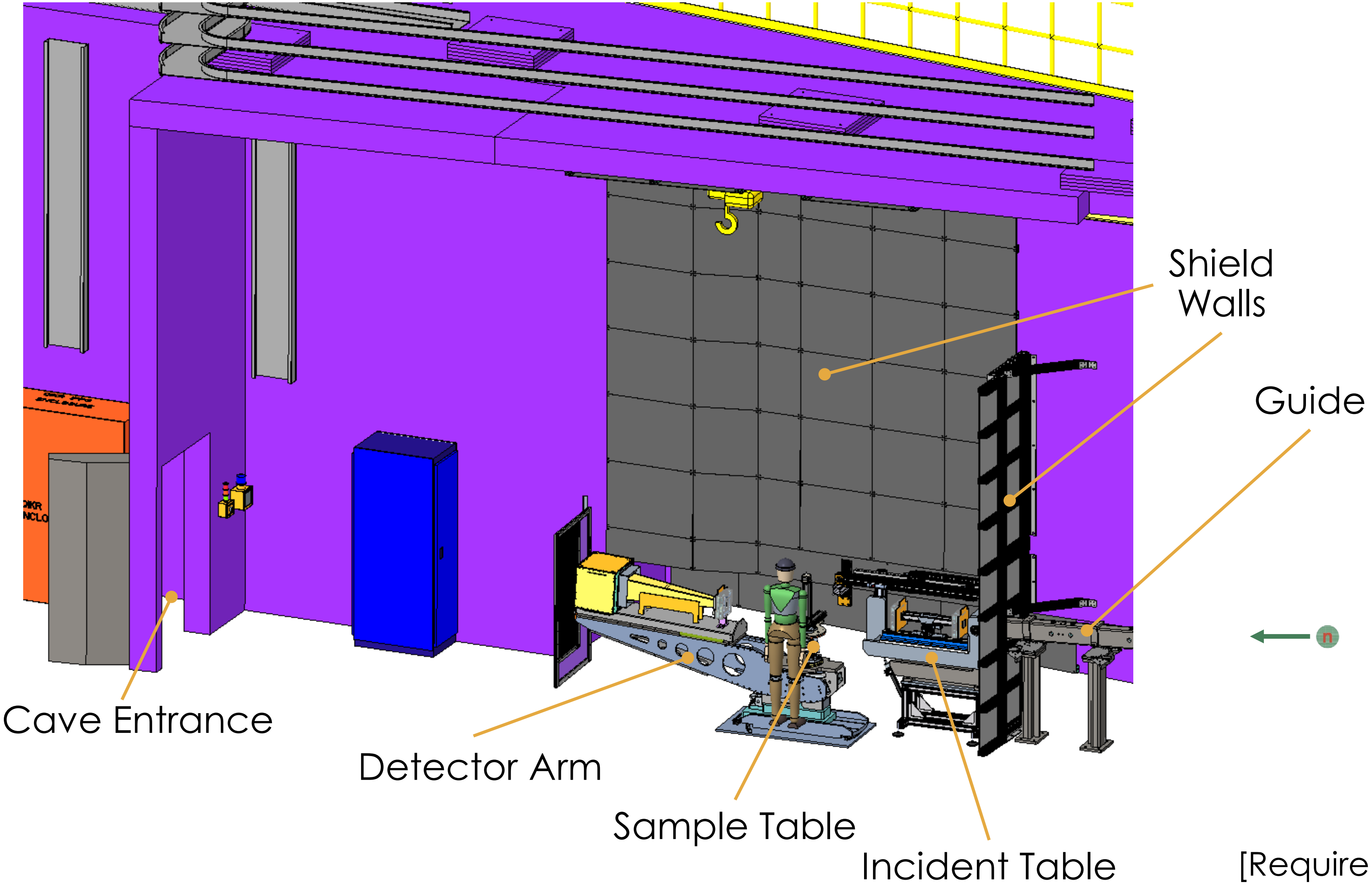
Location of QIKR

QIKR will sit at port ST02 and view the cylinder moderator



STS Beamlines in the South Instrument Hall

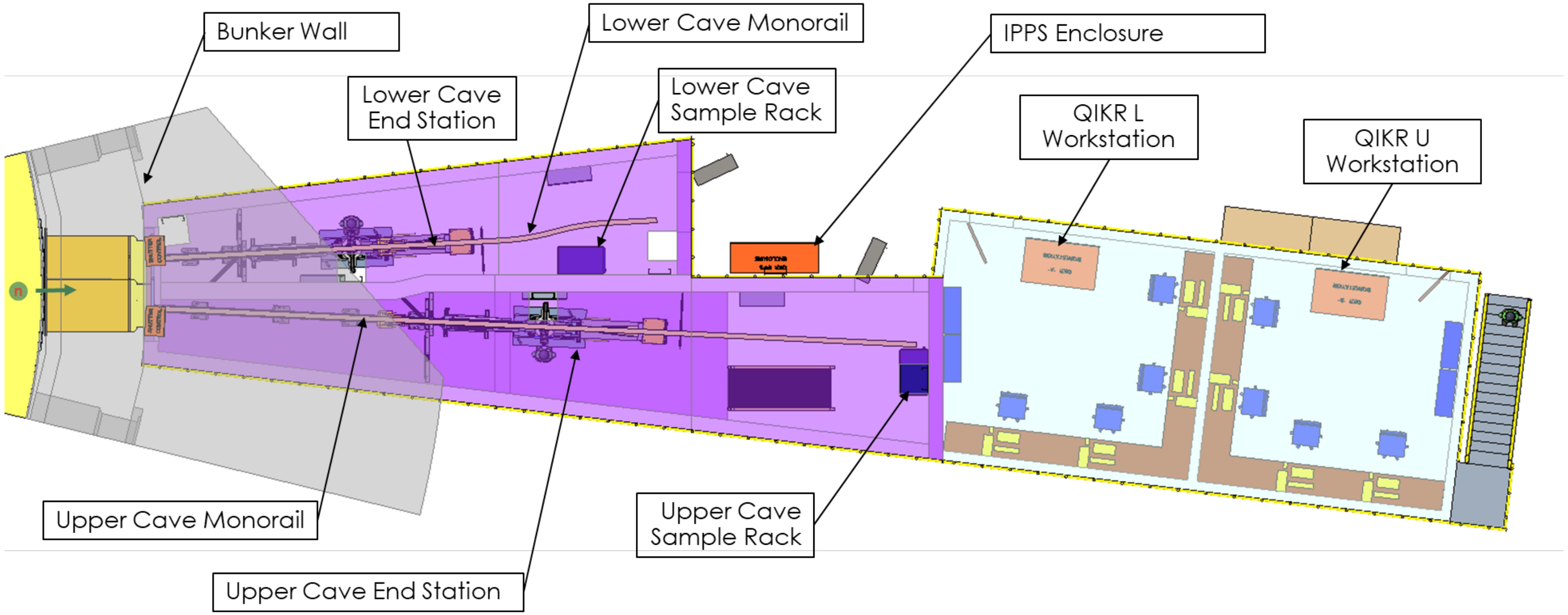
QIKR-L instrument cave



[Requirements A,B,F]

Summary

- The specifications of QIKR instrument motions have been derived from the physical requirements for performing accurate and repeatable reflectivity measurements to fulfill the science mission.
- We have shown here calculations for the most important of these motions.
- These and other requirements have been captured in the QIKR Motion Systems Requirements document (S04080600_SRD10000-R00).



Thanks

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