NOVEL NUMERICAL METHOD FOR CALCULATING THE SHADOW PROJECTION AND COLLISIONS OF A MULTI-AXIS GONIOMETER AT DIAMOND

SHADOWS & COLLISIONS

Beamline I23

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Diamond Light Source, UK

WEAA04

MEDSI 2016
MECHANICAL ENGINEERING DESIGN OF SYNCHROTRON RADIATION EQUIPMENT AND INSTRUMENTATION

14/09/2016

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Beamline I23

- Macromolecular crystallography (MX) beamline using long wavelengths to solve protein structures.

- Wavelength (energy) range:
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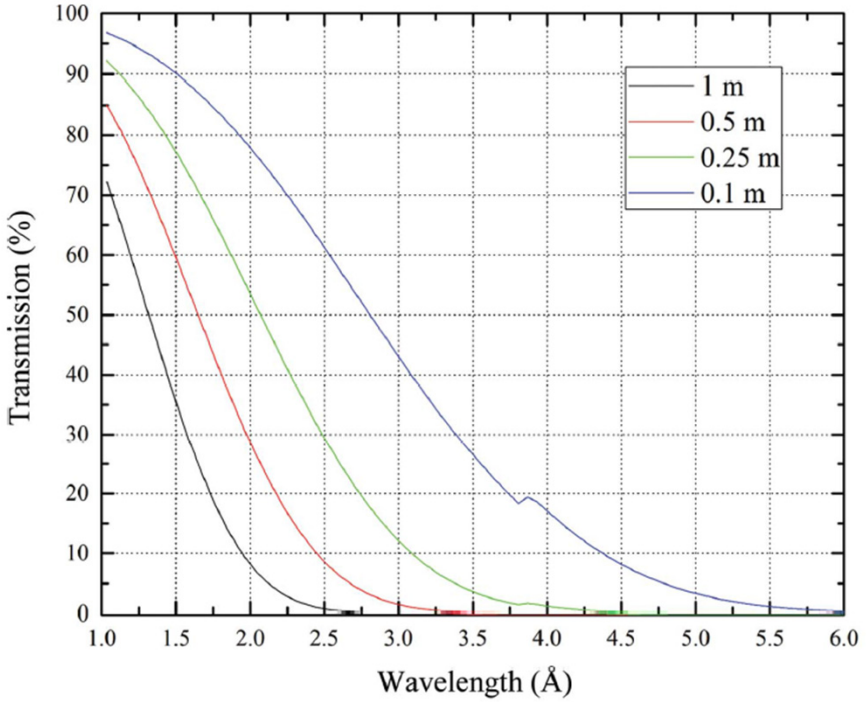

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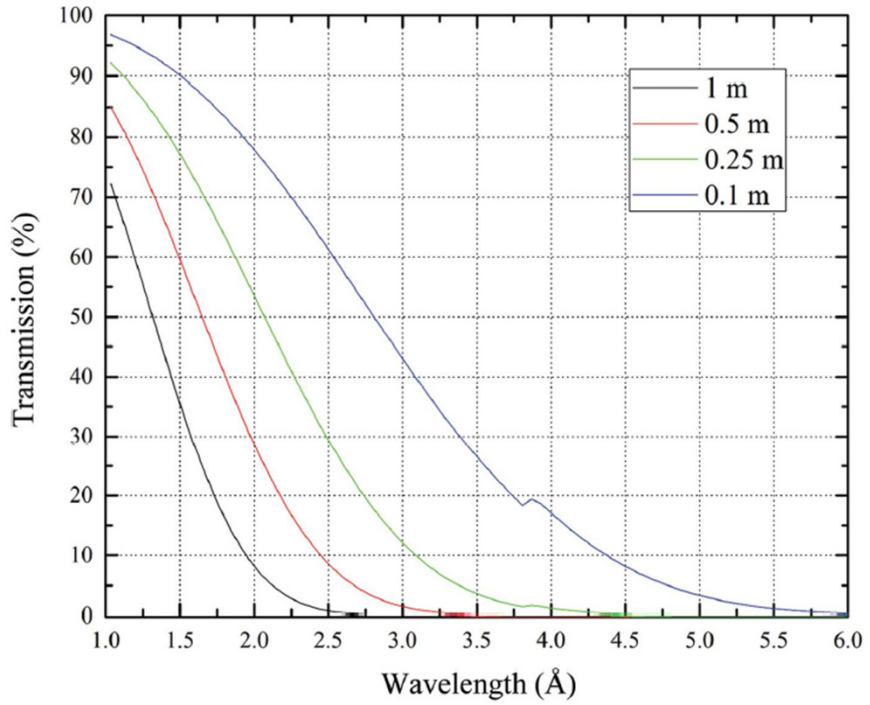
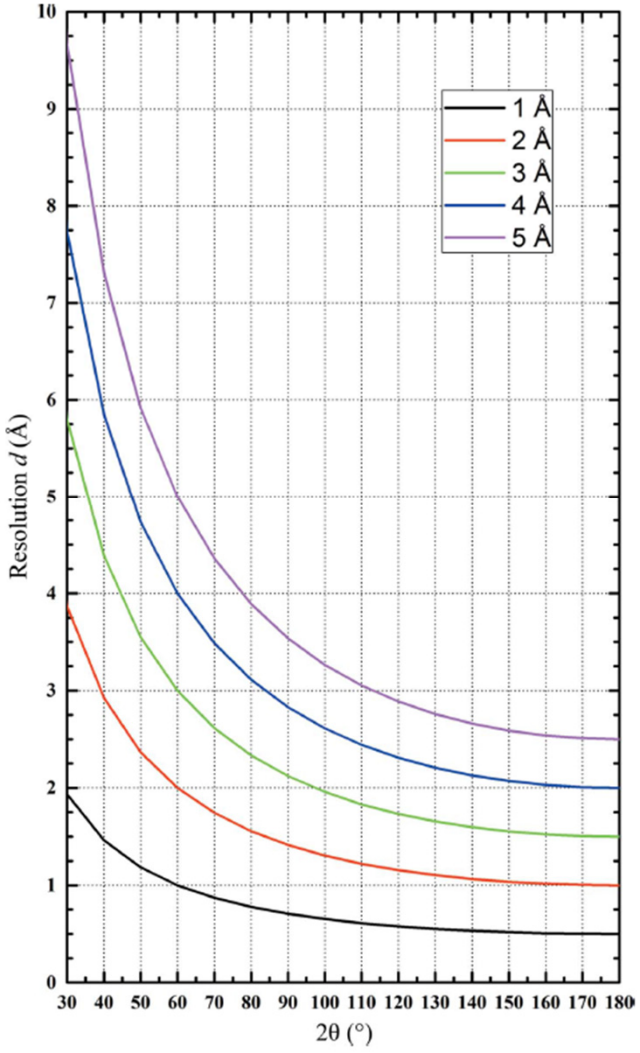


Beamline I23

$d = \lambda / (2 \sin\theta)$



Resolution as function of Bragg angle for different wavelengths.

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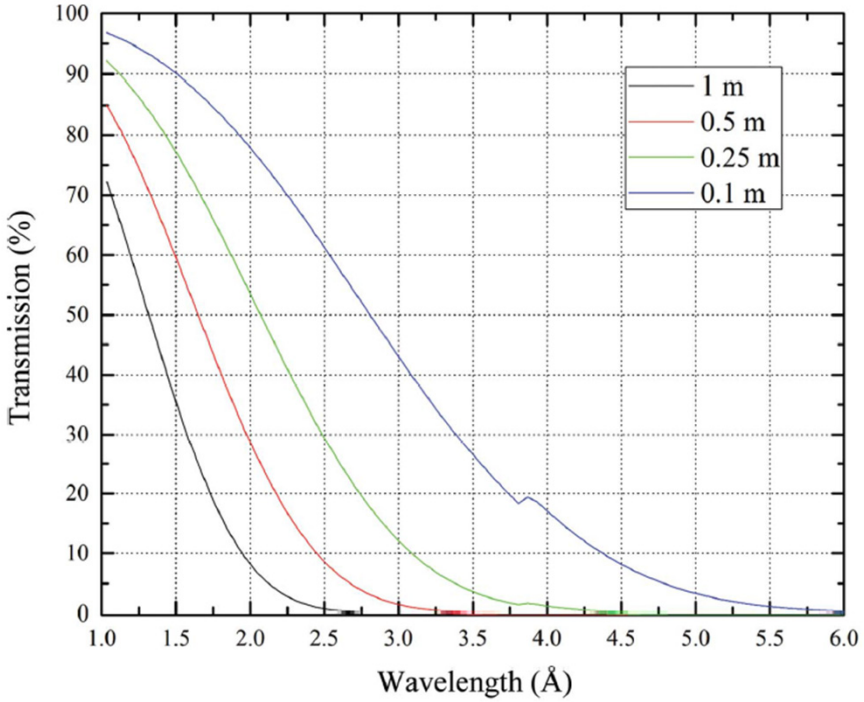
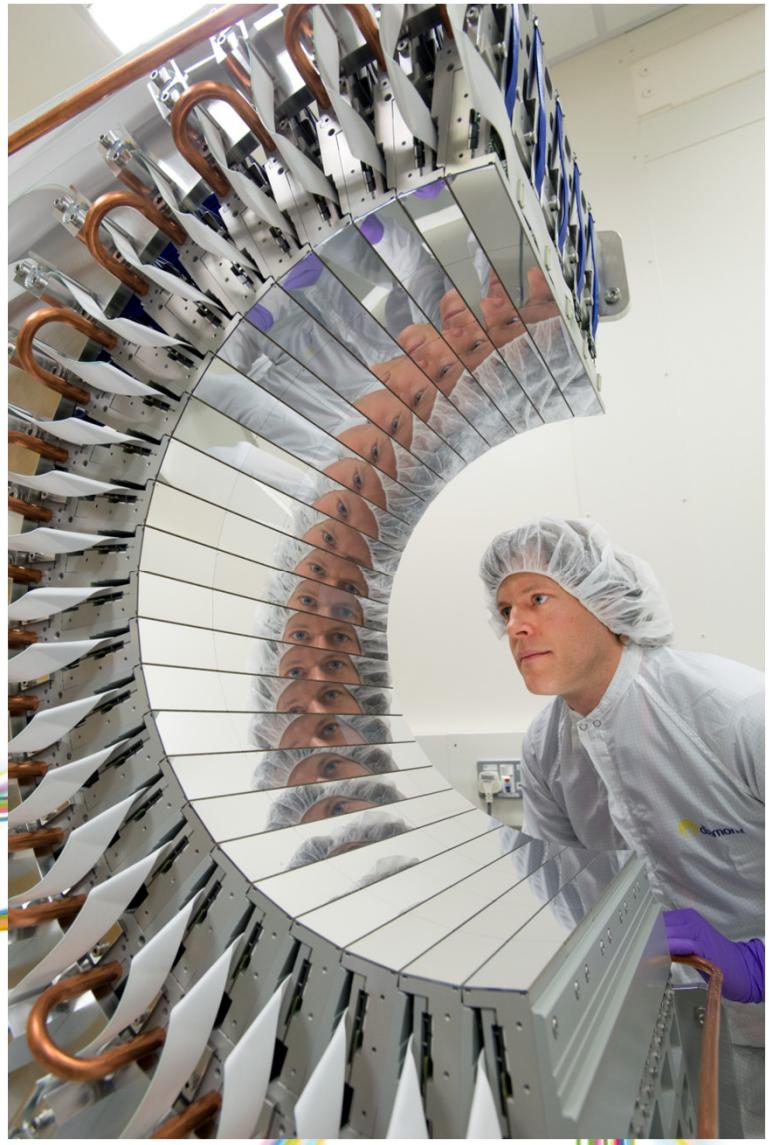
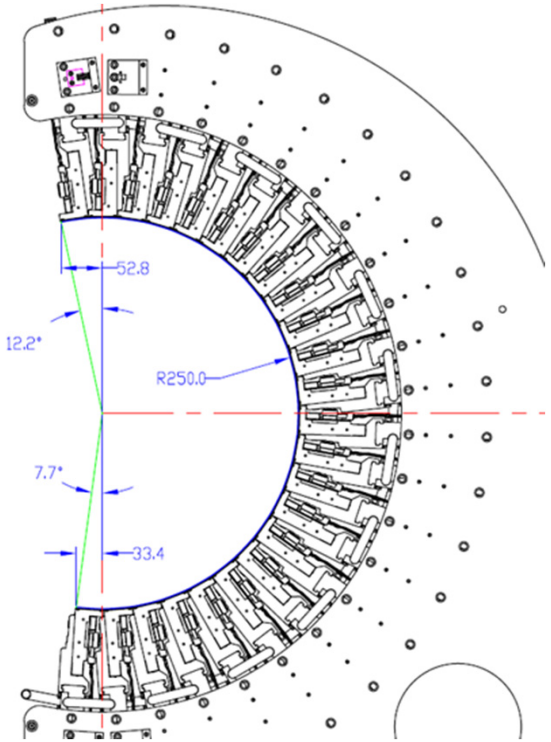


Pilatus 12M

DECTRIS®





- 120 modules in vacuum
- Readout electronics in air
- Half cylinder r = 250 mm
- Width z = 424.6 mm
- 2θ = ±100° (40.3° laterally)

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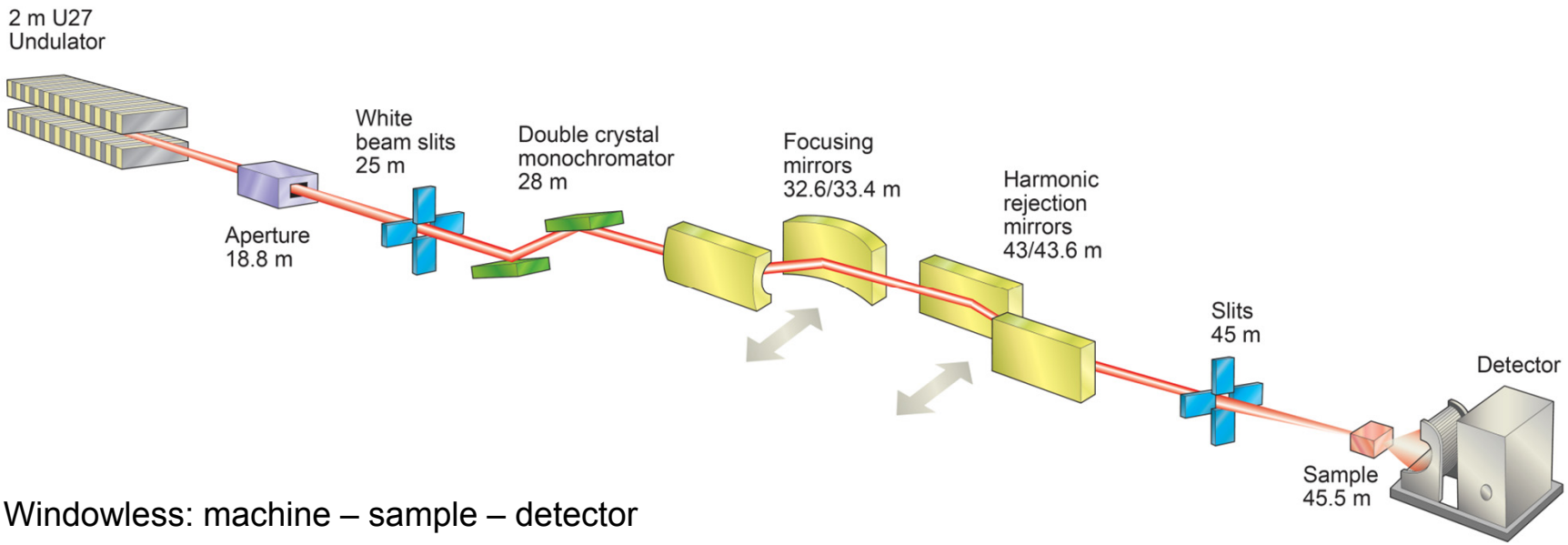
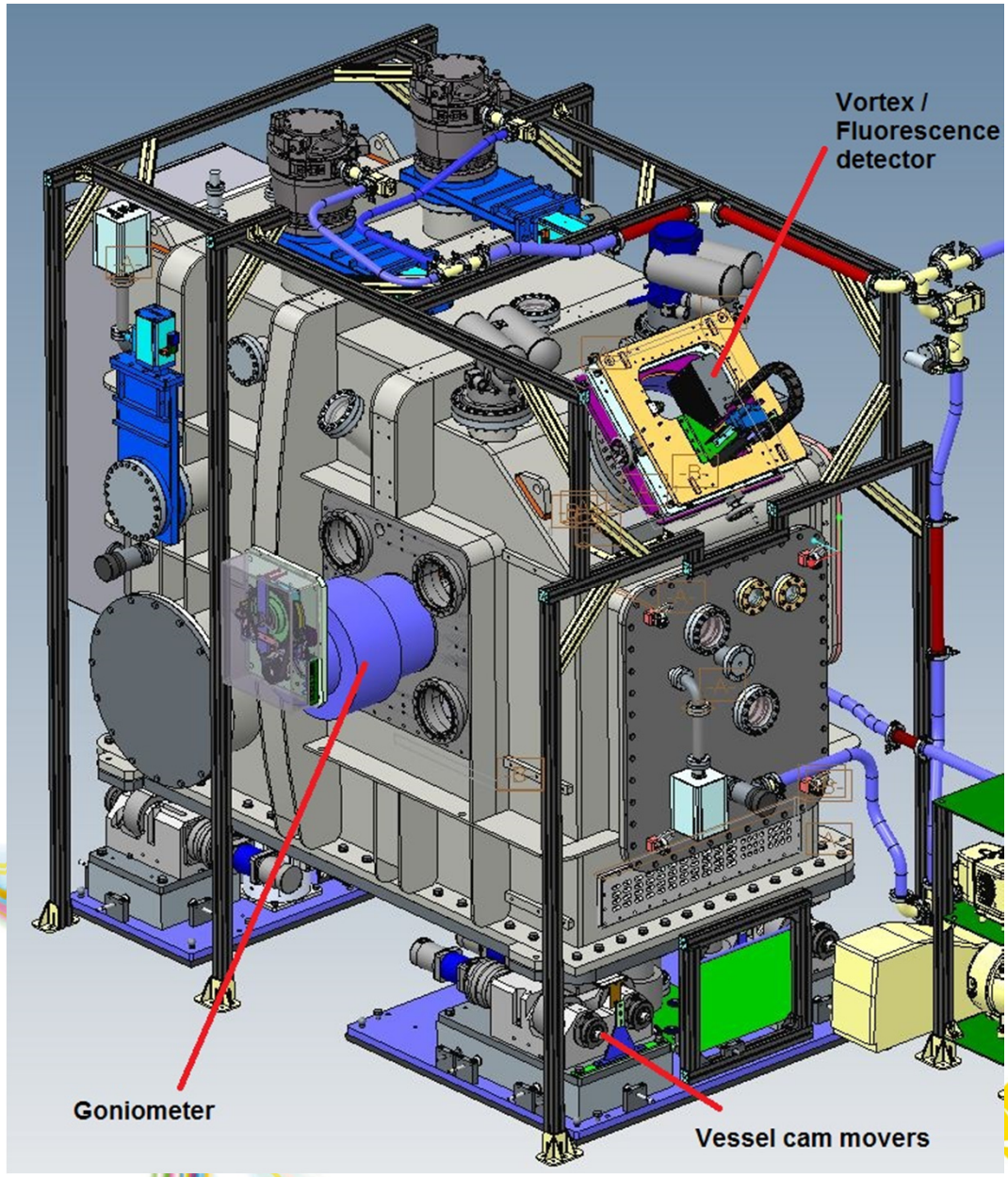
I23 – Long wavelength MX beamline



- Windowless: machine – sample – detector
- Unique end station – experiments conducted in vacuum and at cryogenic temperatures
- Beam size at sample:
  100 - 1000 μm
- Photon flux:
  5 x 10^{12} ph/s in 100 x 100 μm @ 4 keV

I23 – End station



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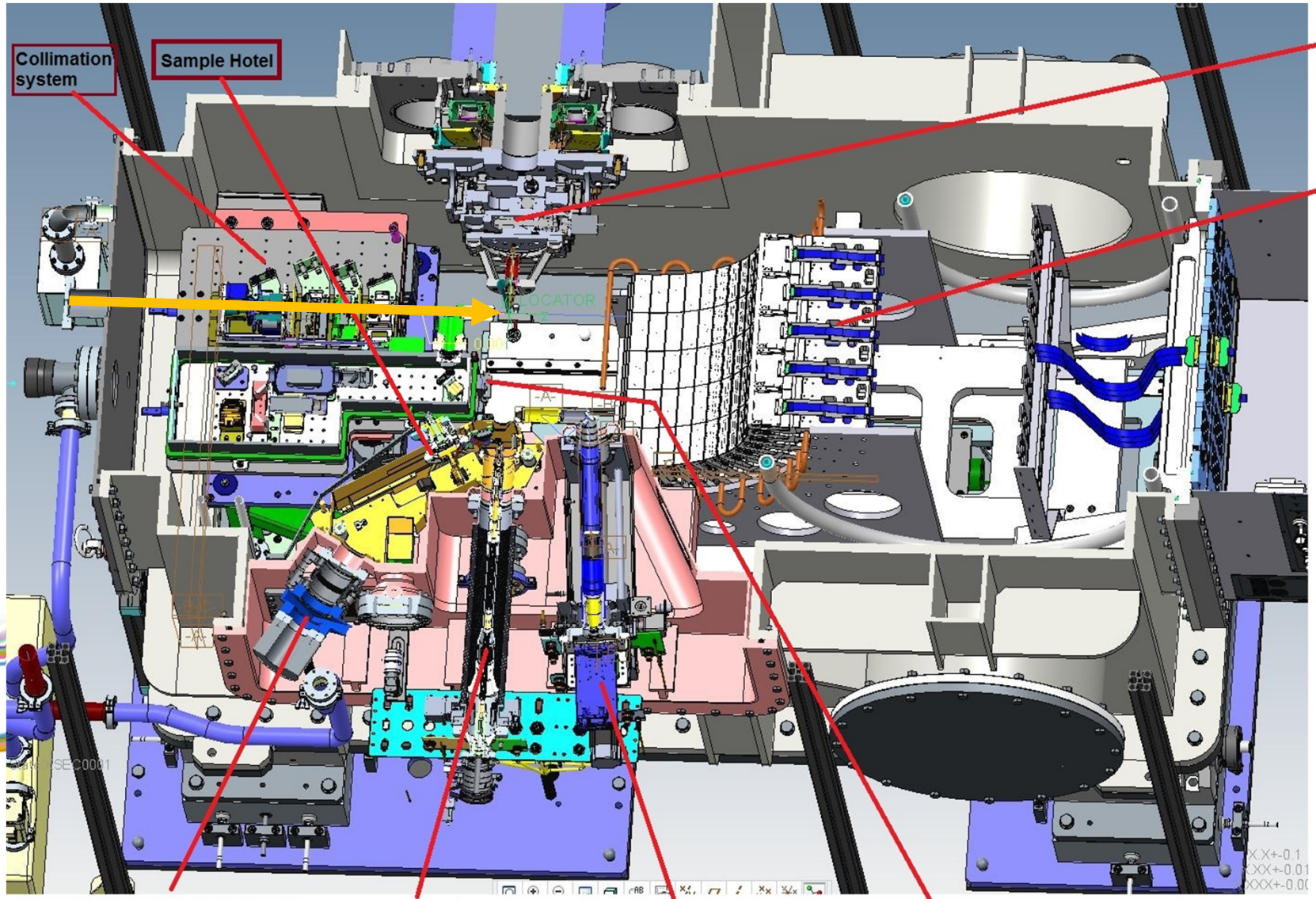
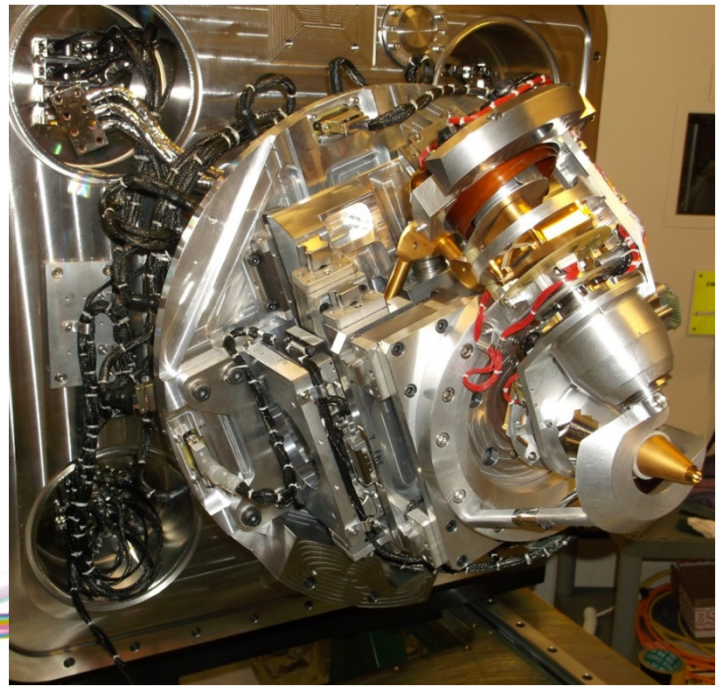
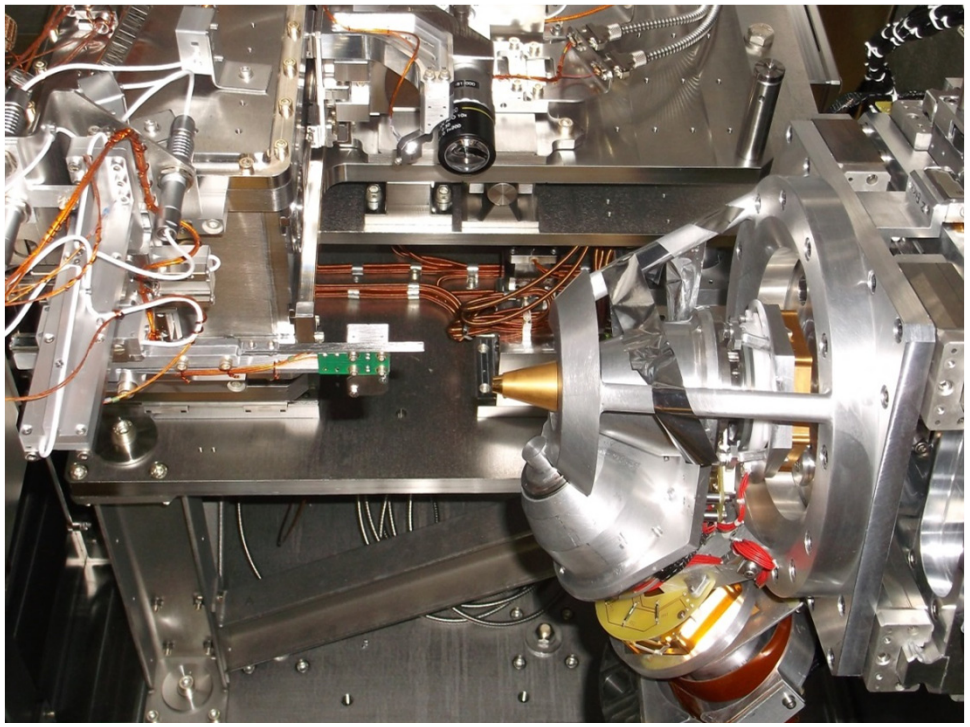


Multi-axis goniometer

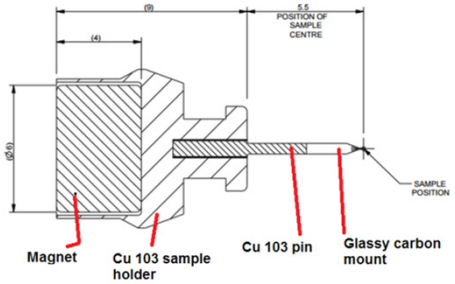
Science & Technology Facilities Council
UK Astronomy Technology Centre

- Commissioned to Astronomy Technology Centre in Edinburgh
- 5 μm sphere of confusion
- Conductive cooling link for sample temperatures 40 – 120 K





- Inverse Kappa geometry ($\propto$ = 50°)
- Omega (ω) axis = ± 270°
- Kappa (κ) axis = -10° to +190°
- Phi (φ) axis = ± 180°
- XYZ = ± 2.5 mm



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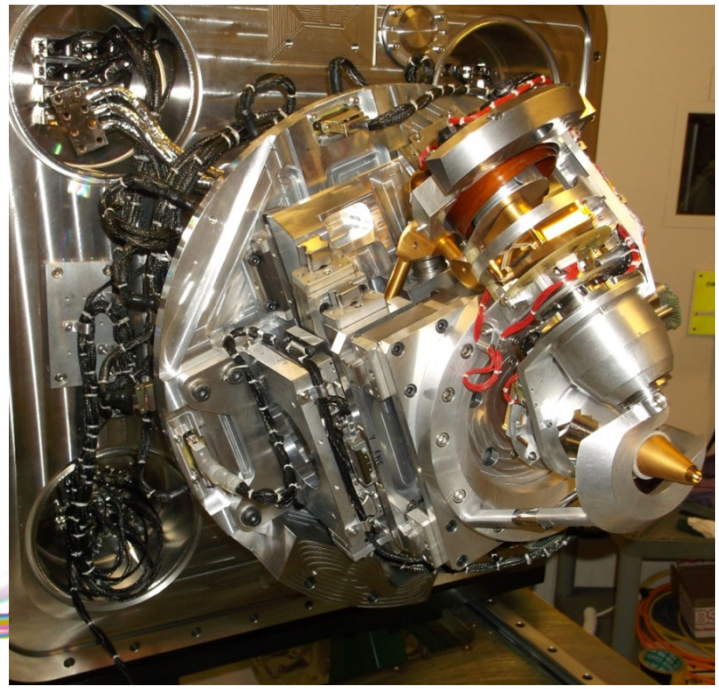

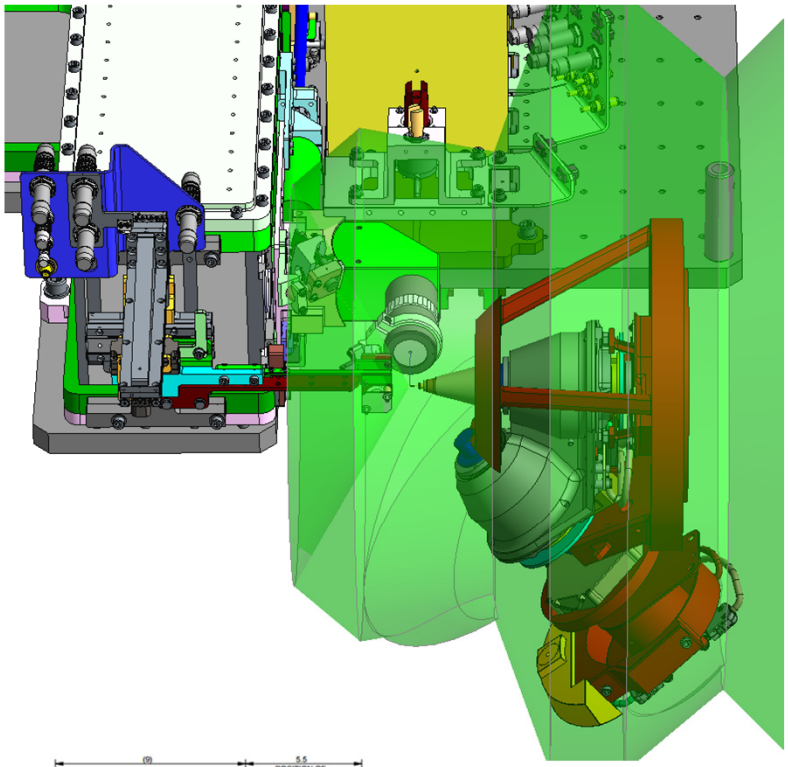

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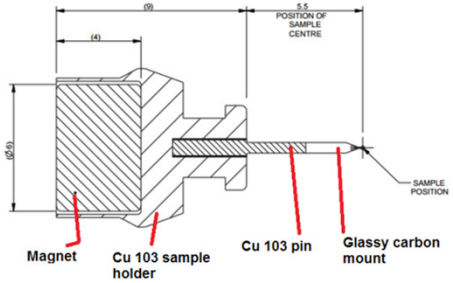

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Optimisation strategy for data collection

- Samples can only be exposed to a certain amount of radiation dose.
- Strategy required to optimally orient the crystal in 3D space for obtaining a complete dataset with minimum X-ray dose.
- Contract - Global Phasing Limited (GΦL) to generate optimisation strategy for data collection.

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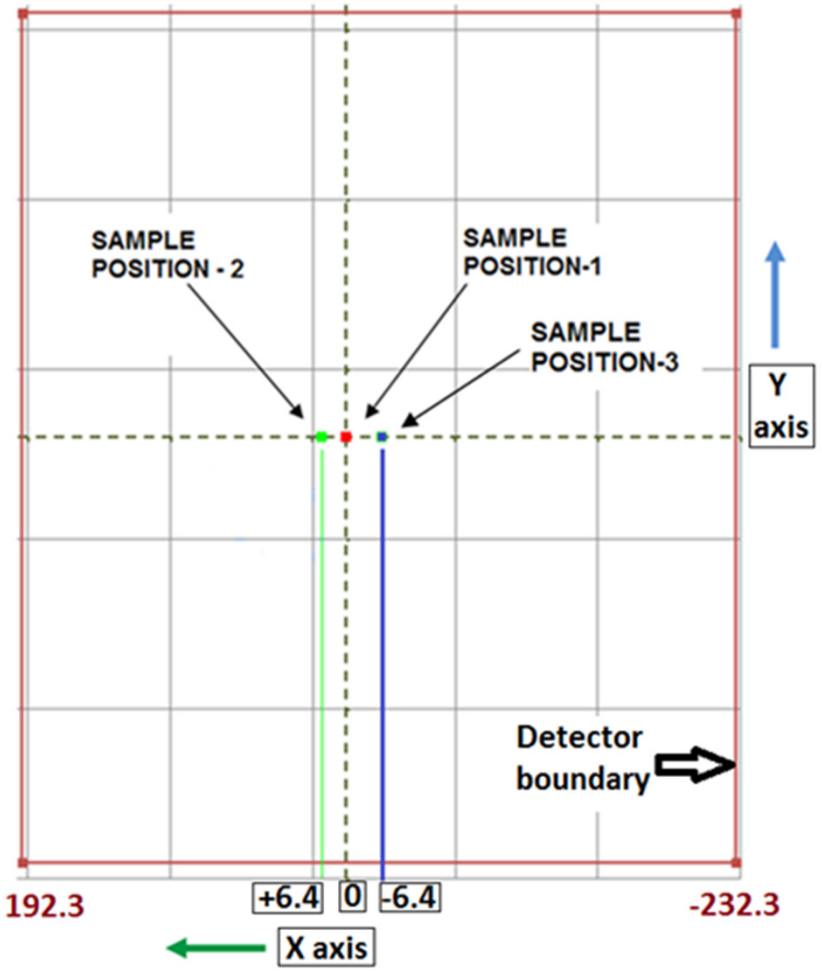
1. **Shadow:** cast on the detector by the goniometer.
2. **Collisions:** Restricting angular range for sample centering and data collection.

Shadow model

Six main factors affect the location and shape of the shadow on the detector –

1. The 3D geometry of the goniometer kappa axis assembly
2. The 3D geometry of the detector
3. The Omega angle
4. The Kappa angle
5. The XYZ offset on the centering stage
6. The Sample position



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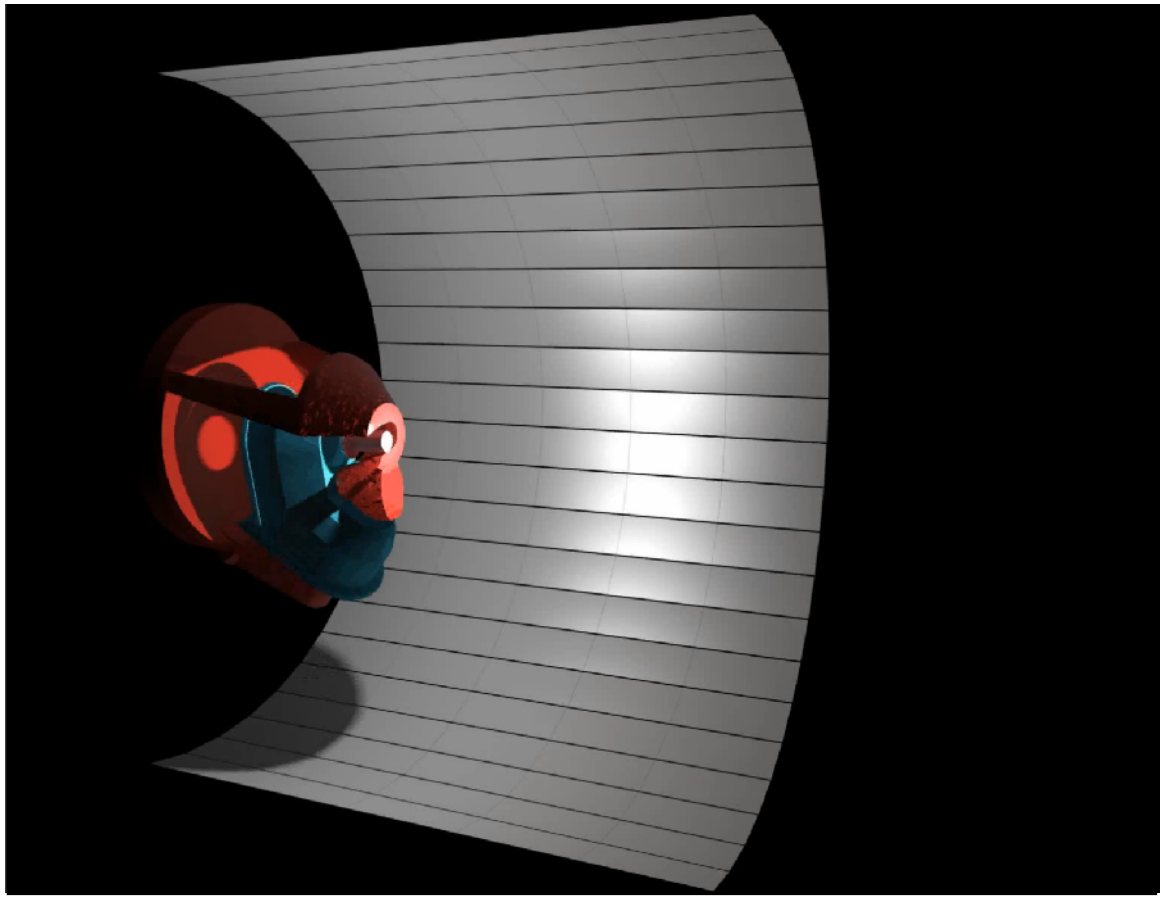

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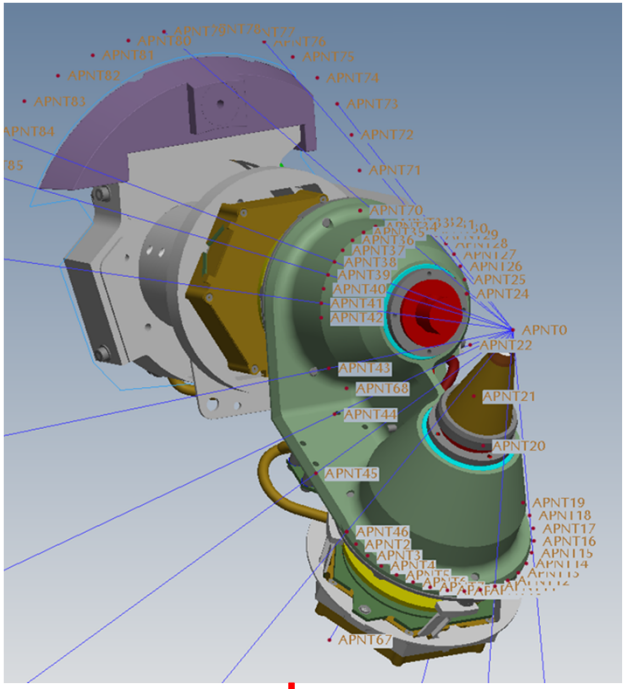

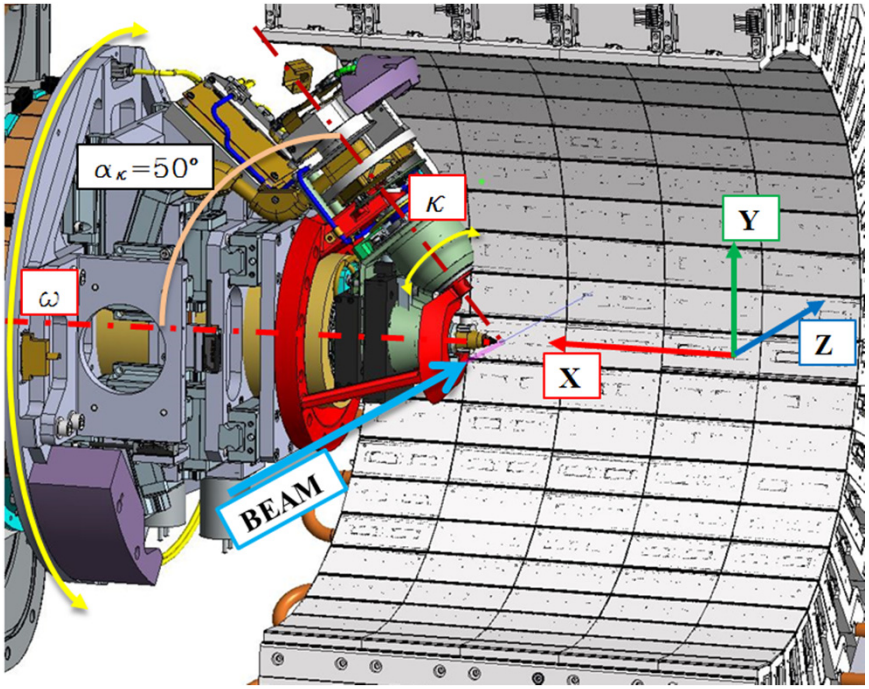

$$C_G = \begin{bmatrix} X_1 & Y_1 & Z_1 \\ \vdots & \ddots & \vdots \\ X_n & Y_n & Z_n \end{bmatrix}$$

$$R_K = \begin{bmatrix} u^2 + v^2\cos\kappa & uv(1-\cos\kappa) & -v\sin\kappa \\ uv(1-\cos\kappa) & v^2 + u^2\cos\kappa & +u\sin\kappa \\ +v\sin\kappa & -u\sin\kappa & (u^2+v^2)\cos\kappa \end{bmatrix}$$

$$u = \cos\ (50^0)$$
$$v = \sin\ (50^0)$$

$$[C_{KG}] = [C_G] \times [R_K]$$

Offset in XYZ

$$R_\omega = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\omega & \sin\omega \\ 0 & -\sin\omega & \cos\omega \end{bmatrix}$$

$$[C_{\omega G}] = [C_{KO}] \times [R_\omega]$$

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Shadow model

Ray –

Origin point H (x_h, y_h, z_h)

Offset vector I (x_i, y_i, z_i)

Equation of a ray –

$$P(t) = G + t(I),\ t>0$$

$[C_{\omega G}]$ →

$$x(t) = t.x_i$$
$$y(t) = t.y_i$$
$$z(t) = t.z_i$$

Equation of a cylinder of infinite length along the X-axis with a radius = 250 –

$$z^2 + y^2 = 250^2$$

↓

$$t = \frac{\pm\sqrt{[-(4(z_i^2 + y_i^2)(-(250^2))]}}{2(z_i^2 + y_i^2)}$$

Detector – partial-cylinder of finite length. X and Z coordinates valid if –

- For sample position – 1: -232.3 mm < x < 192.3 mm and z > -52.8 mm (i.e., -12^0 < **w** < 190^0)
- For sample position – 2: -238.7 mm < x < 185.9 mm and z > -52.8 mm (i.e., -12^0 < **w** < 190^0)
- For sample position – 3: -225.9 mm < x < 198.7 mm and z > -52.8 mm (i.e., -12^0 < **w** < 190^0)

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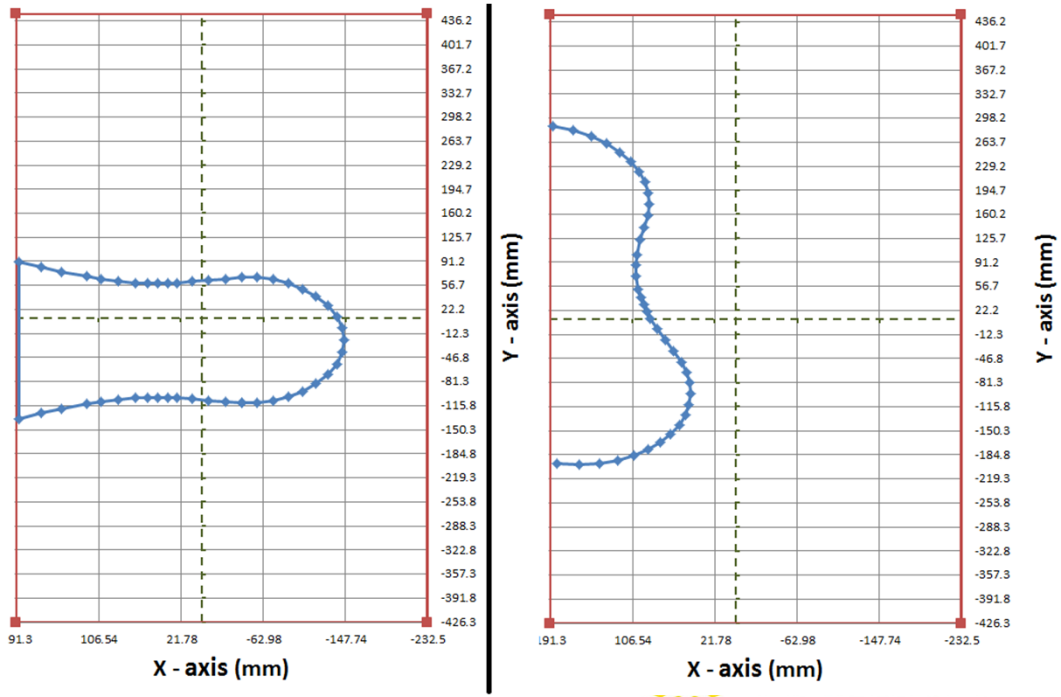

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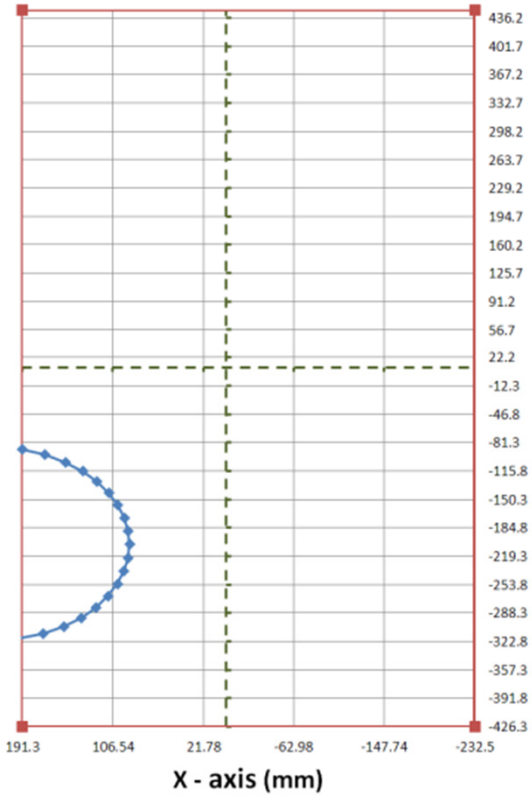
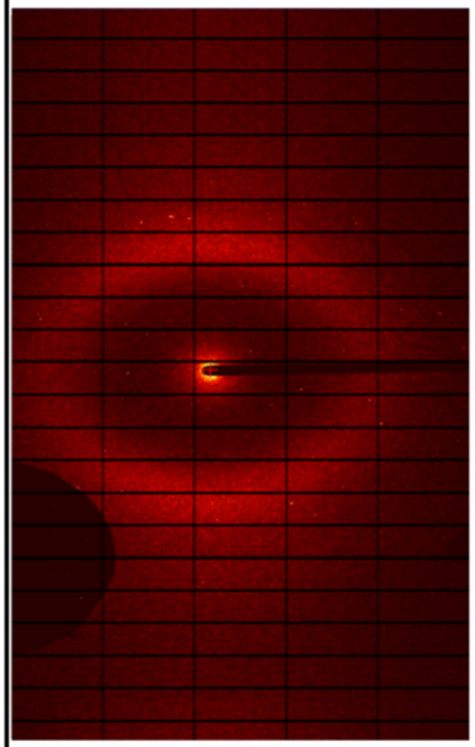
Shadow projected on detector surface (front view)



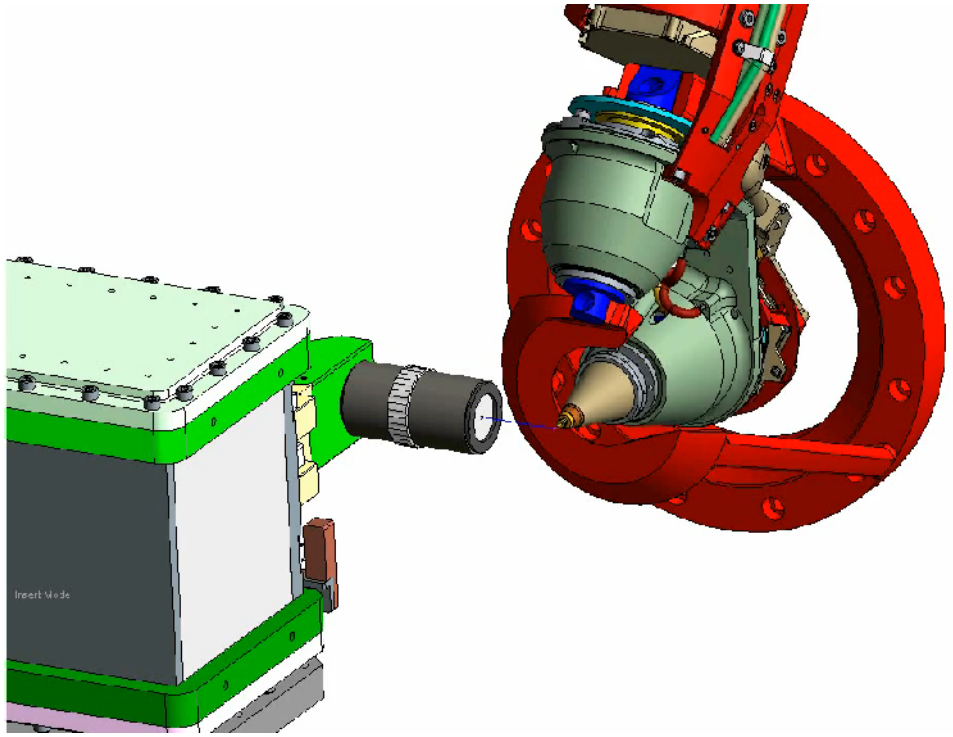
ω = 137.6° ; κ = -10°



Collision model

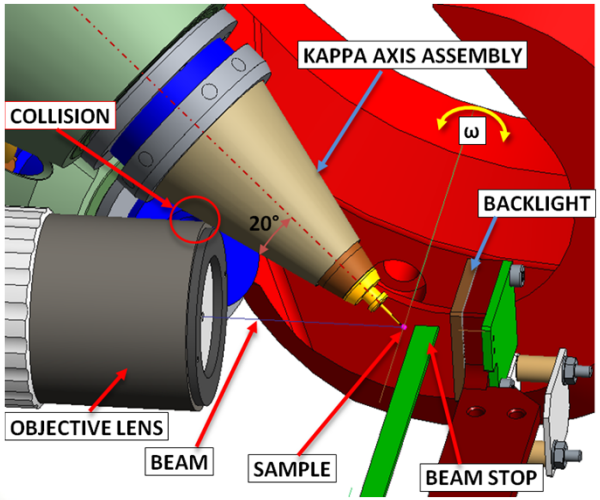
Collisions –

1. **Sample centering**: Kappa axis assembly, objective lens and backlight.
2. **Data collection**: Kappa axis assembly and beam stop.



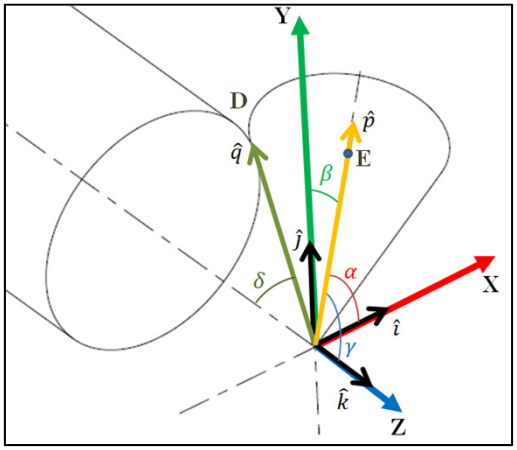
Collisions dependent on –

1. The Kappa angle
2. The Omega angle
3. The XYZ centering offsets on the goniometer centering stage.
4. The distance of the objective lens from the sample position in the Z direction.
5. The distance of the backlight from the sample position in the Z direction.
6. The distance of the beam stop from the sample position in the Z direction.
7. The geometry of the colliding parts.



Collision model

Objective



$$A_C = \begin{bmatrix} 0 & 0 & 0 \\ x_E & y_E & z_E \end{bmatrix}$$

$$[A_{KC}] = [A_C] \times [R_K]$$

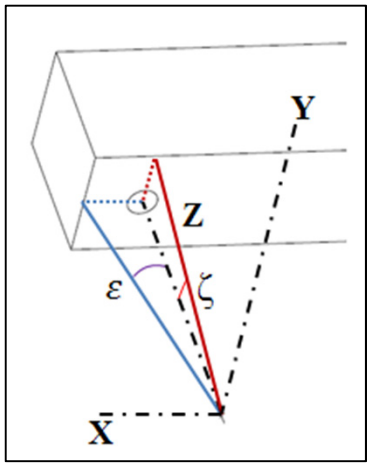
$$[A_{\omega C}] = [A_{KC}] \times [R_\omega] = \begin{bmatrix} 0 & 0 & 0 \\ x_{E1} & y_{E1} & z_{E1} \end{bmatrix}$$

$$\gamma_{\omega C} = \pi - \left(\cos^{-1} \left(\frac{z_{E1}}{\sqrt{(x_{E1}^2 + y_{E1}^2 + z_{E1}^2)}} \right) \right)$$

Collision if,

$\gamma_{\omega C}$ (in degrees) $\leq$ δ + 20°

Beam stop



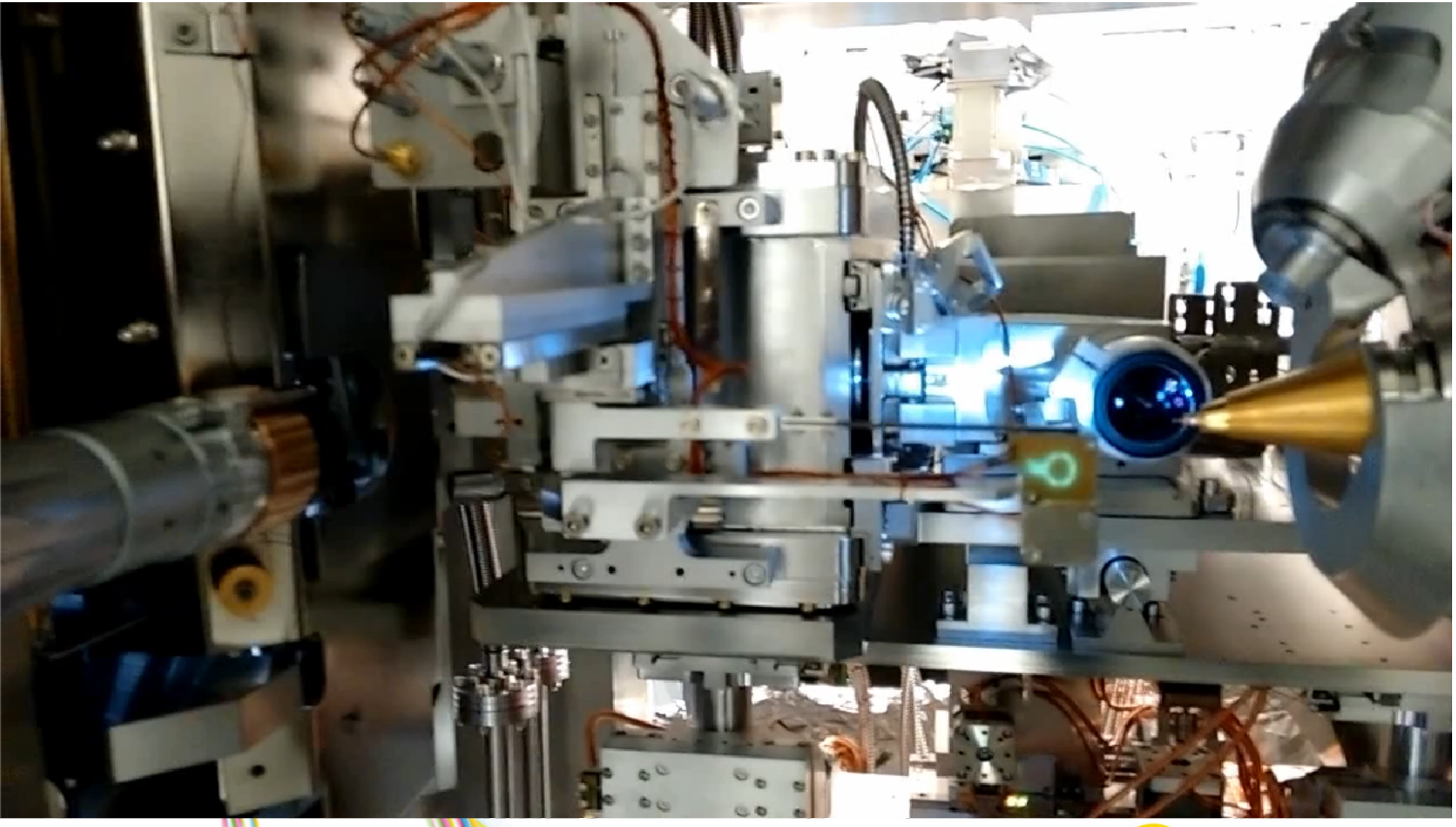
Angle between kappa cone axis ($\hat{p}$) and X plane (α) – constant for all omega

- $\hat{p}_x$ – projection vector on YZ plane
- θk – angle between the projected vector and the Y-axis (omega 0°)

Collision if,

- α + 20° is greater than or equal to 90° - ε
- & omega is between - (ζ + θk + 20°) & (ζ - θk + 20°)

Collision model testing



Conclusion

- Collision model – tested and is accurate. Additional safety margins added.
- Shadow model – visually compared against a few recorded images on the detector and is a good match. Detailed analysis is yet to be performed.
- Models can be easily adapted for other installations – has been done for the SmarGon with shadowing on a flat Pilatus 6M detector.

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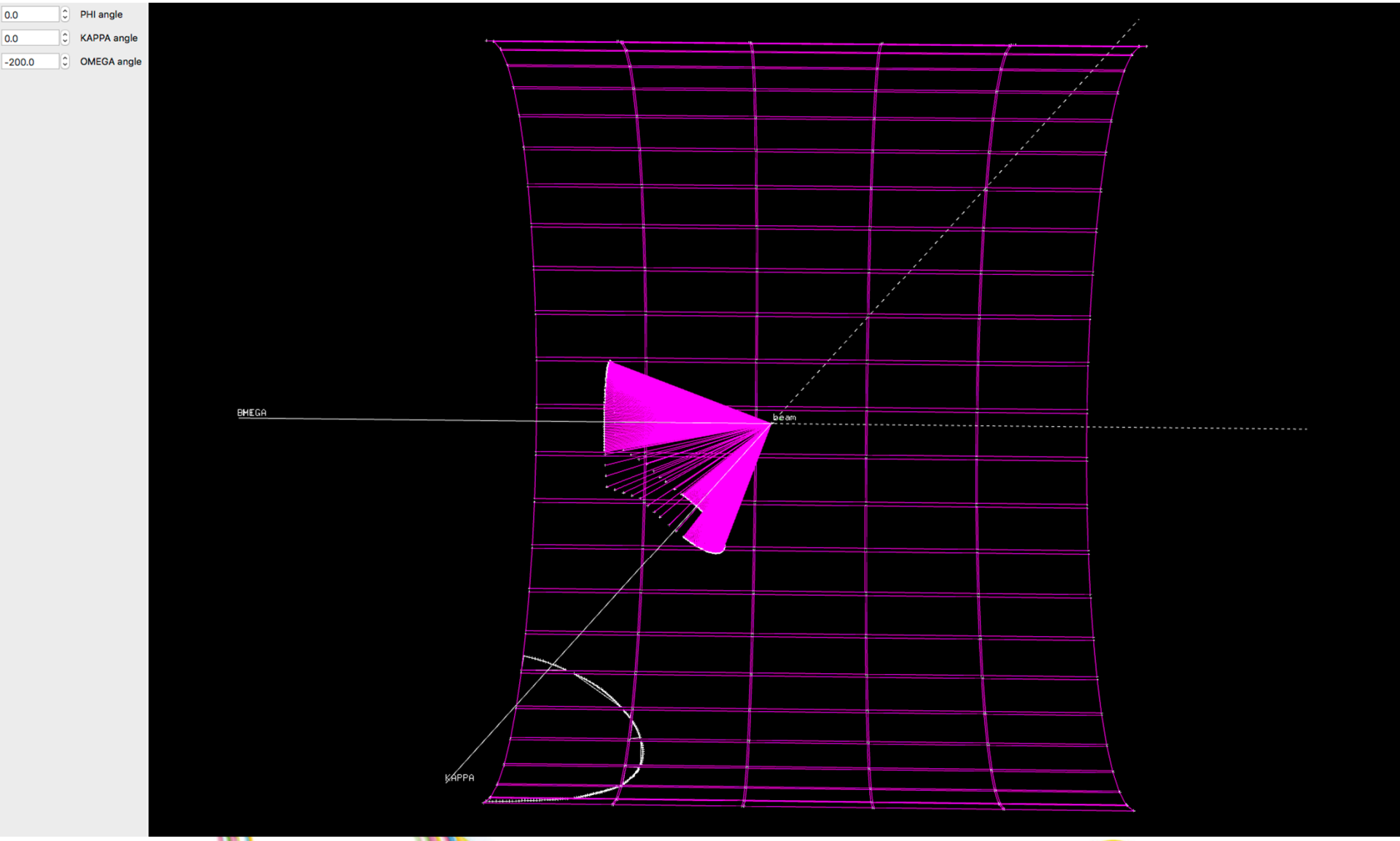
Thank you

Q & A

Shadow model (DIALS: Diffraction Integration for Advanced Light Sources)



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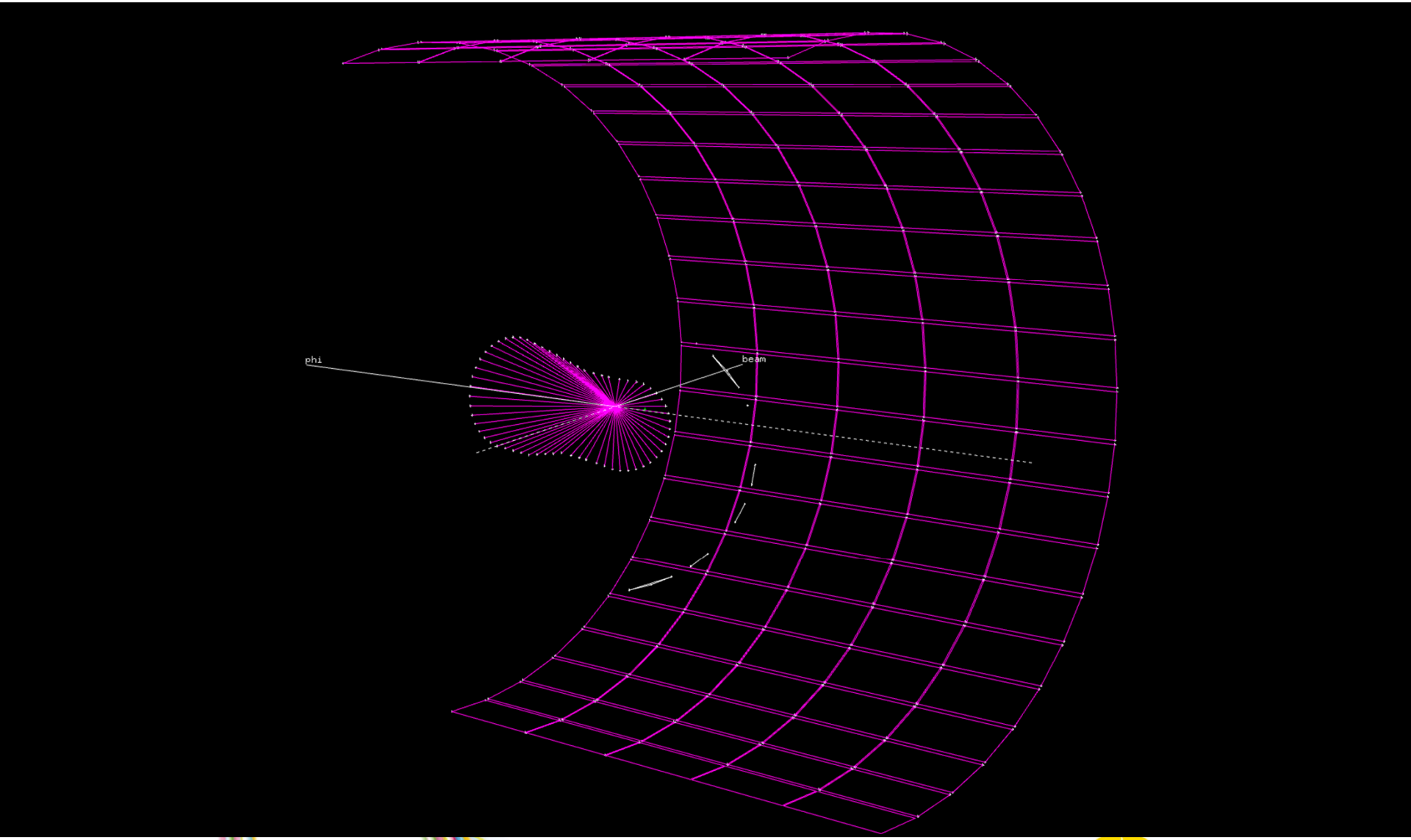

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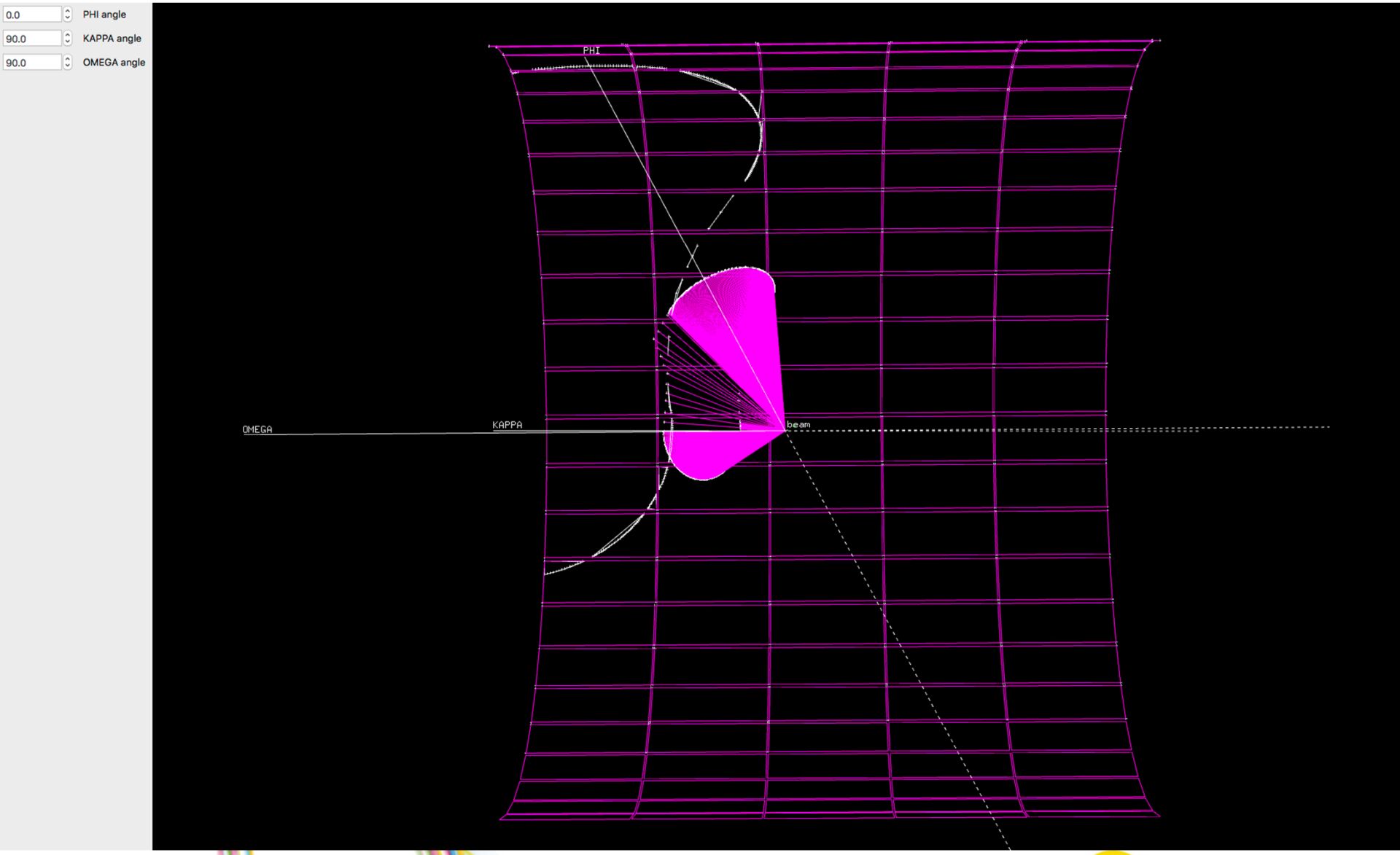

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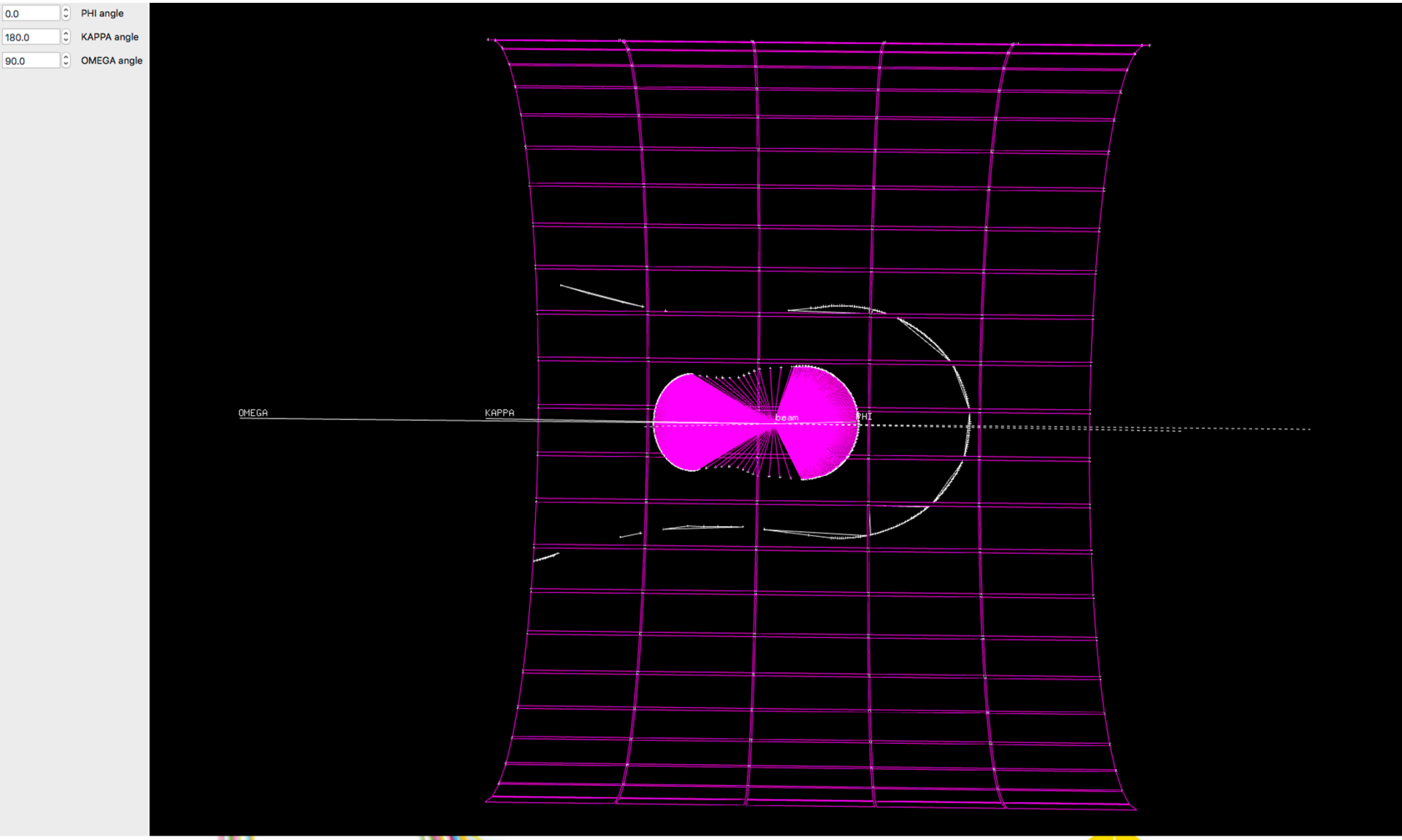
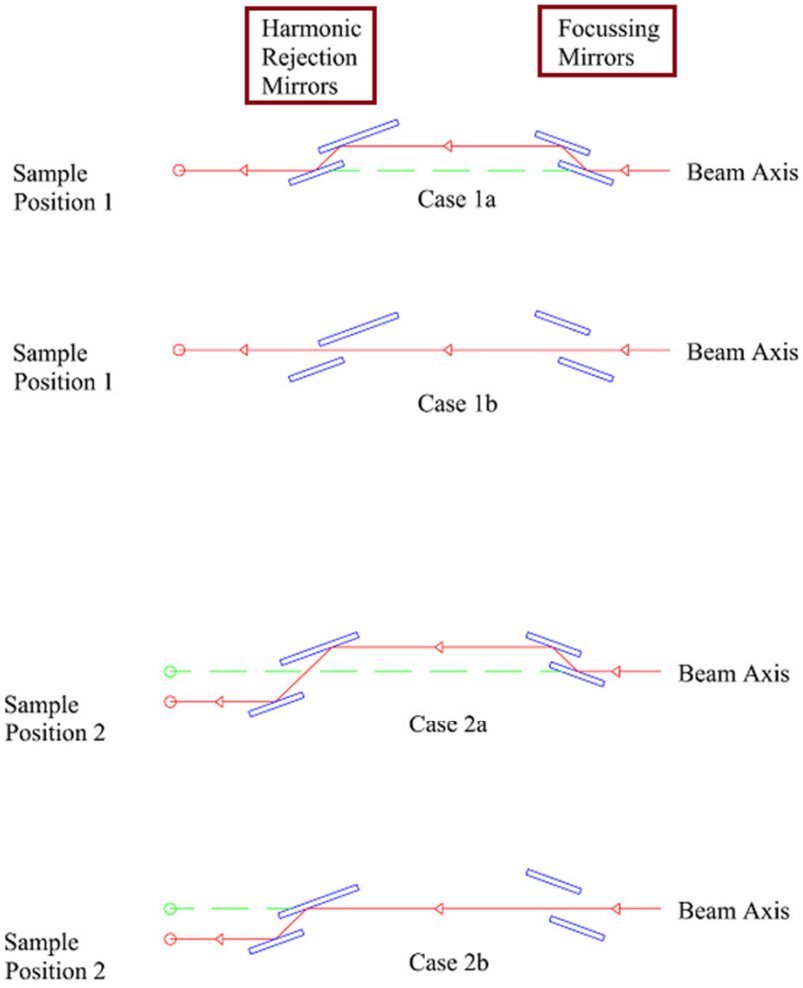


Sample positions



Schematic view of mirror configurations (plan view).

Mode	F mirrors	HR mirrors	Remarks
1a	In	In	Exit beams for case 1a and case 1b coincide and are in line with the undeflected beam from the DCM.
1b	Out	Out	
2a	In	In	Exit beams for case 2a and case 2b coincide but are offset from the undeflected beam from the DCM.
2b	Out	In	

Offset\Mode	1A	1B	2A	2B
DCM – FM	-6.4	0	-6.4	0
DCM - HMR	0	0	+6.4	+6.4

Sample positions

Viewport views