TOSCA Secondary Spectrometer Upgrade: Design & Simulations

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ISIS Neutron and Muon Source

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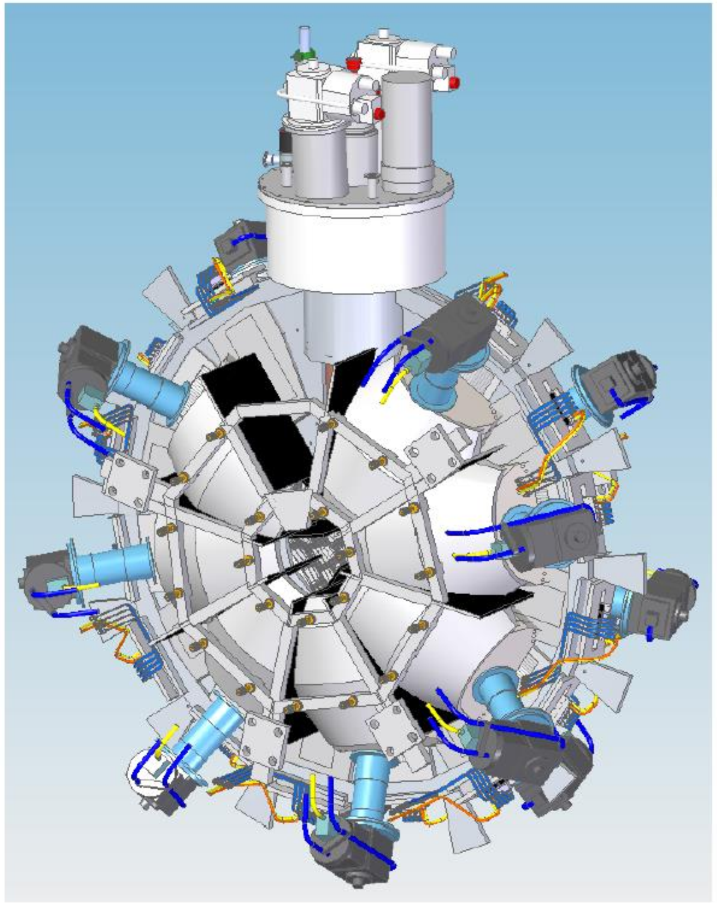
Introduction

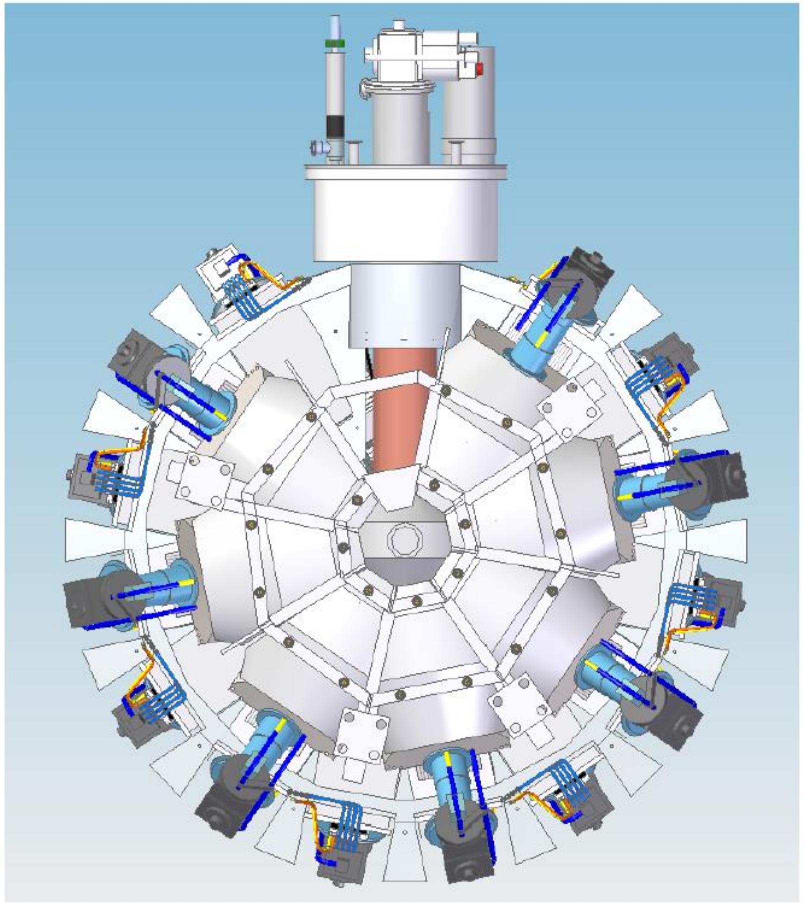
TOSCA+ design process

- **Choice of the assembly**
- **Parameterised analyser**
- **Detector system**
- **Beryllium filter**

Performance comparison

Conclusions





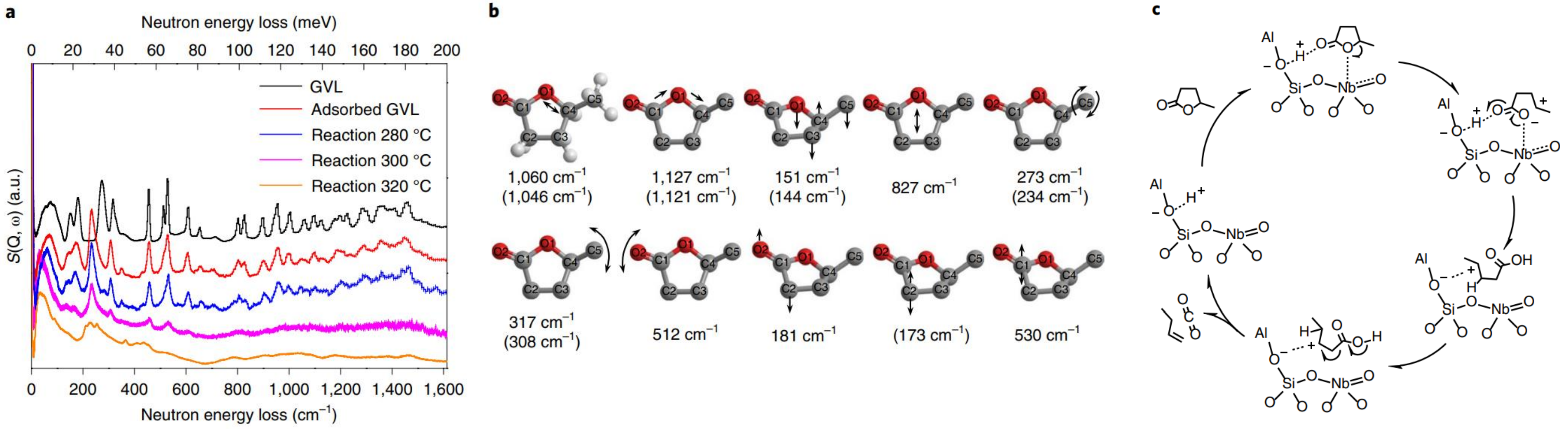
Neutron vibrational spectroscopy (NVS)

- Neutron analogue to infrared/Raman
- “Fingerprint” region: 400–1500 cm^{-1} (50–185 meV), best accessed with indirect-geometry instruments
- Studies of catalysts, hydrogen storage materials, hydrogen bonded systems, advanced materials, biological and organic compounds

ARTICLES
https://doi.org/10.1038/s41563-019-0562-6
nature materials

Quantitative production of butenes from biomass-derived γ-valerolactone catalysed by hetero-atomic MFI zeolite

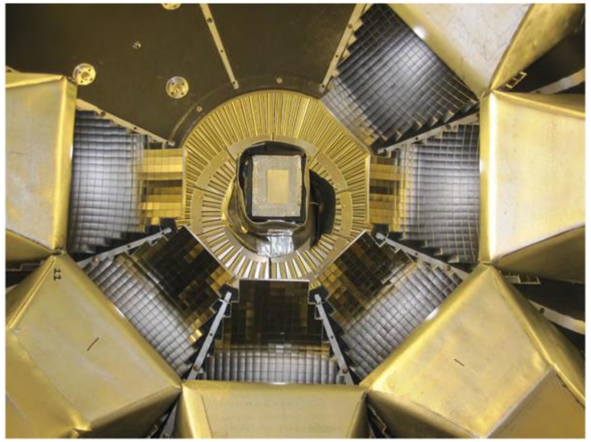
Longfei Lin[1], Alena M. Sheveleva[1,2], Ivan da Silva[3], Christopher M. A. Parlett[4,5,6], Zhimou Tang[7], Yueming Liu[7], Mengtian Fan[1], Xue Han[1], Joseph H. Carter[1], Floriana Tuna[1], Eric J. L. McInnes[1], Yongqiang Cheng[8], Luke L. Daemen[8], Svemir Rudić[3], Anibal J. Ramirez-Cuesta[8], Chiu C. Tang[6] and Sihai Yang[1*]



Indirect-geometry spectrometers for NVS

Operational instruments

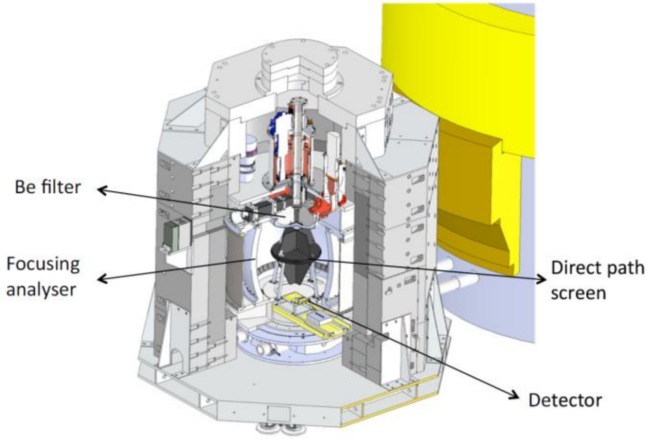
- TOSCA @ISIS, UK
- VISION @ SNS, USA
- LAGRANGE @ILL, France
- NERA @FLNP, Russia



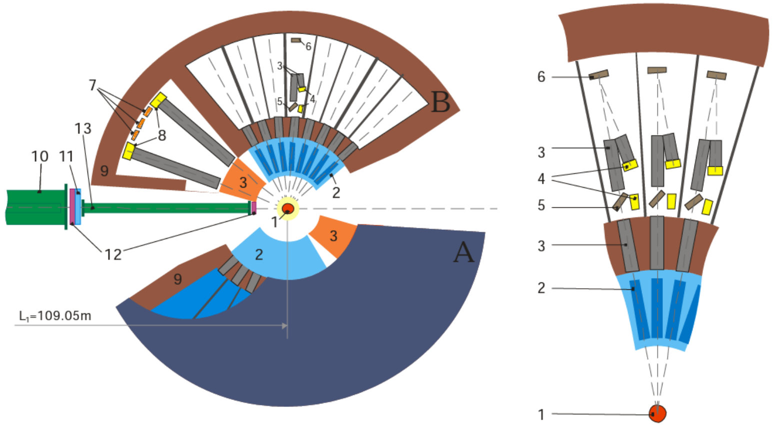
- VISION, https://neutrons.ornl.gov/vision
- Seeger et al., Nucl. Instrum. Methods Phys. Res. A. **604** (2009) 719

Upcoming instruments & upgrades

- TOSCA+ @ISIS, UK
- VESPA @ESS, Sweden
- IGMVS @CSNS, China
- BJN @FLNP, Russia
- BWAVES @STS, USA



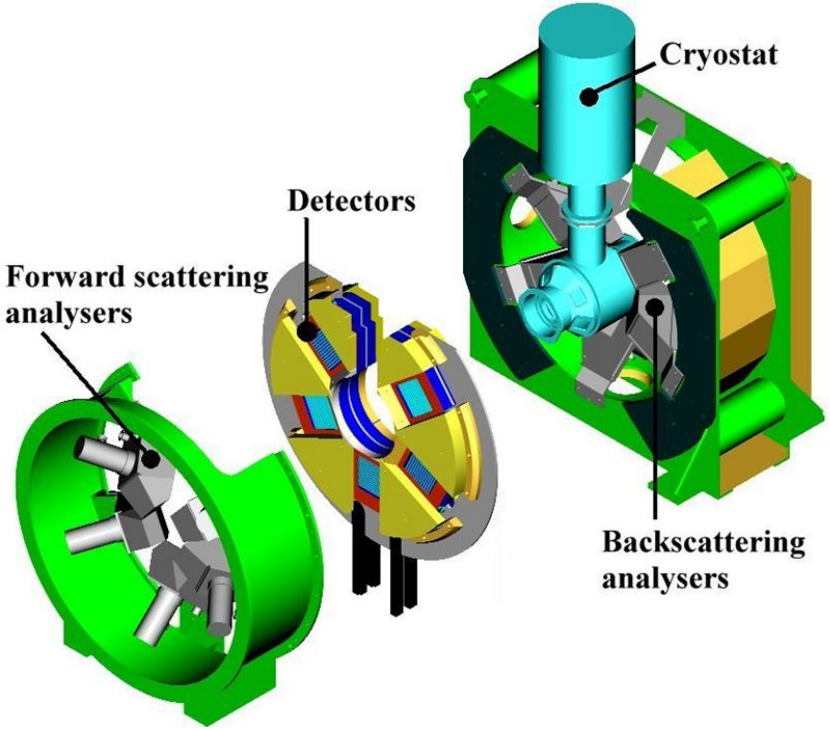
- LAGRANGE, Jiménez-Ruiz et al., J. Phys. Conf. Ser. **549** (2014) 012004



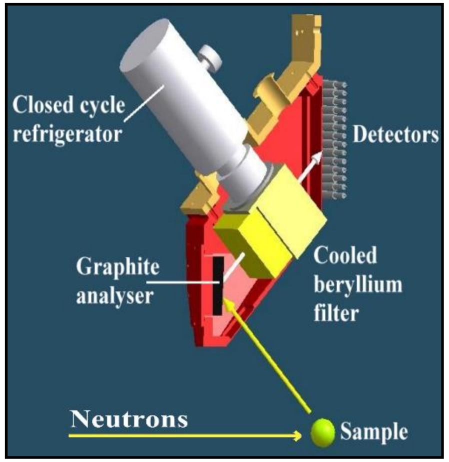
- NERA, Natkaniec et al., J. Phys. Conf. Ser. **554** (2014) 012002

TOSCA secondary spectrometer

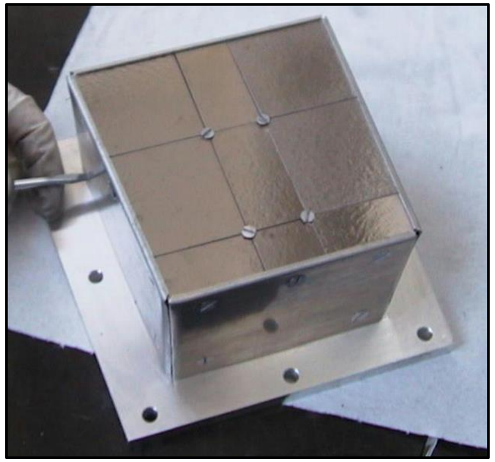
- 5 forward analyser modules
- 5 backward analyser modules
- 1 sr total analyser coverage



Detail of the analyser module



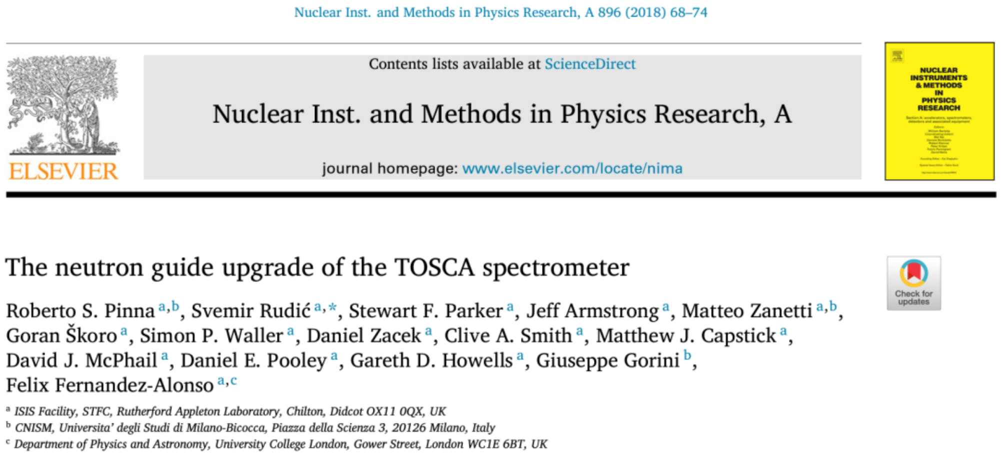
Beryllium filter



Pyrolytic graphite (PG) crystal analyser

Squashed ^{3}He tubes

TOSCA primary spectrometer (upgraded in 2017)


Nuclear Inst. and Methods in Physics Research, A 896 (2018) 68–74

Contents lists available at ScienceDirect

Nuclear Inst. and Methods in Physics Research, A

journal homepage: www.elsevier.com/locate/nima

The neutron guide upgrade of the TOSCA spectrometer

Roberto S. Pinna [a,b], Svemir Rudić [a,*], Stewart F. Parker [a], Jeff Armstrong [a], Matteo Zanetti [a,b], Goran Škoro [a], Simon P. Waller [a], Daniel Zacek [a], Clive A. Smith [a], Matthew J. Capstick [a], David J. McPhail [a], Daniel E. Pooley [a], Gareth D. Howells [a], Giuseppe Gorini [b], Felix Fernandez-Alonso [a,c]

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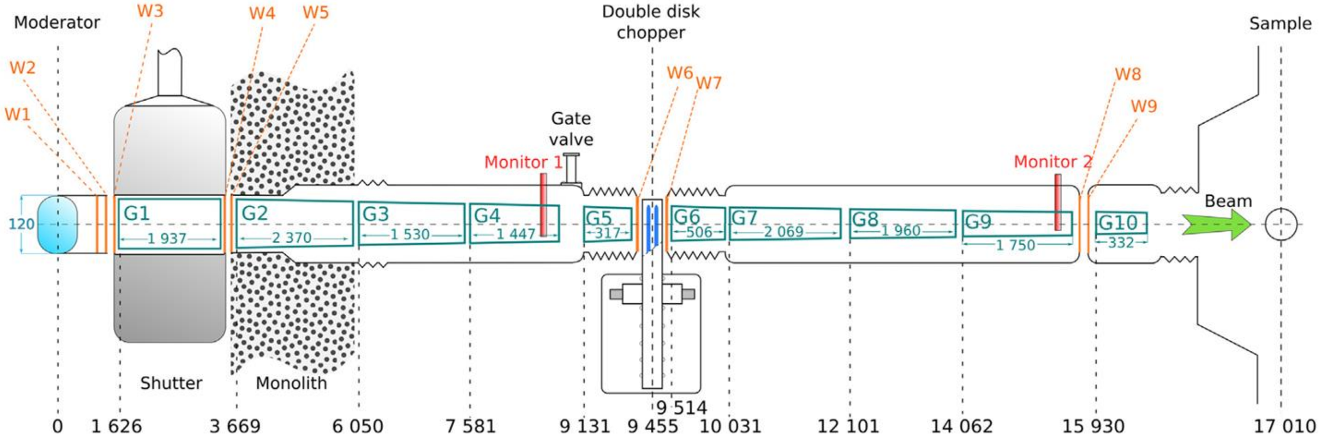
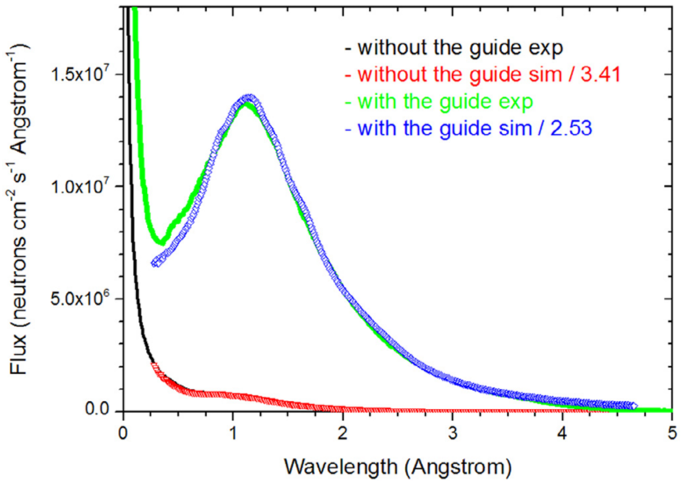
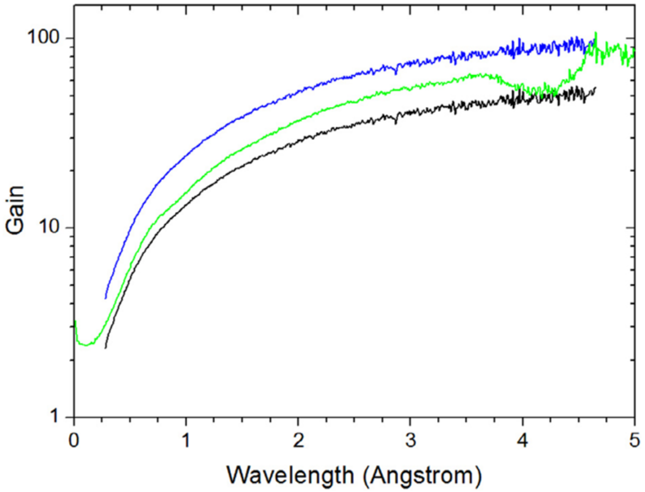
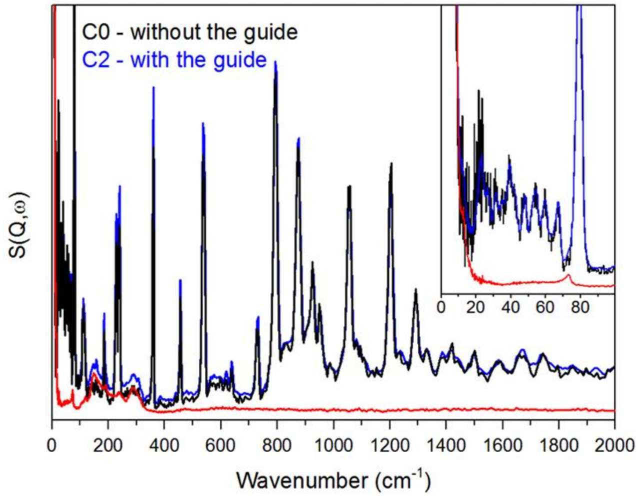
[b] CNISM, Universita' degli Studi di Milano-Bicocca, Piazza della Scienza 3, 20126 Milano, Italy
[c] Department of Physics and Astronomy, University College London, Gower Street, London WC1E 6BT, UK



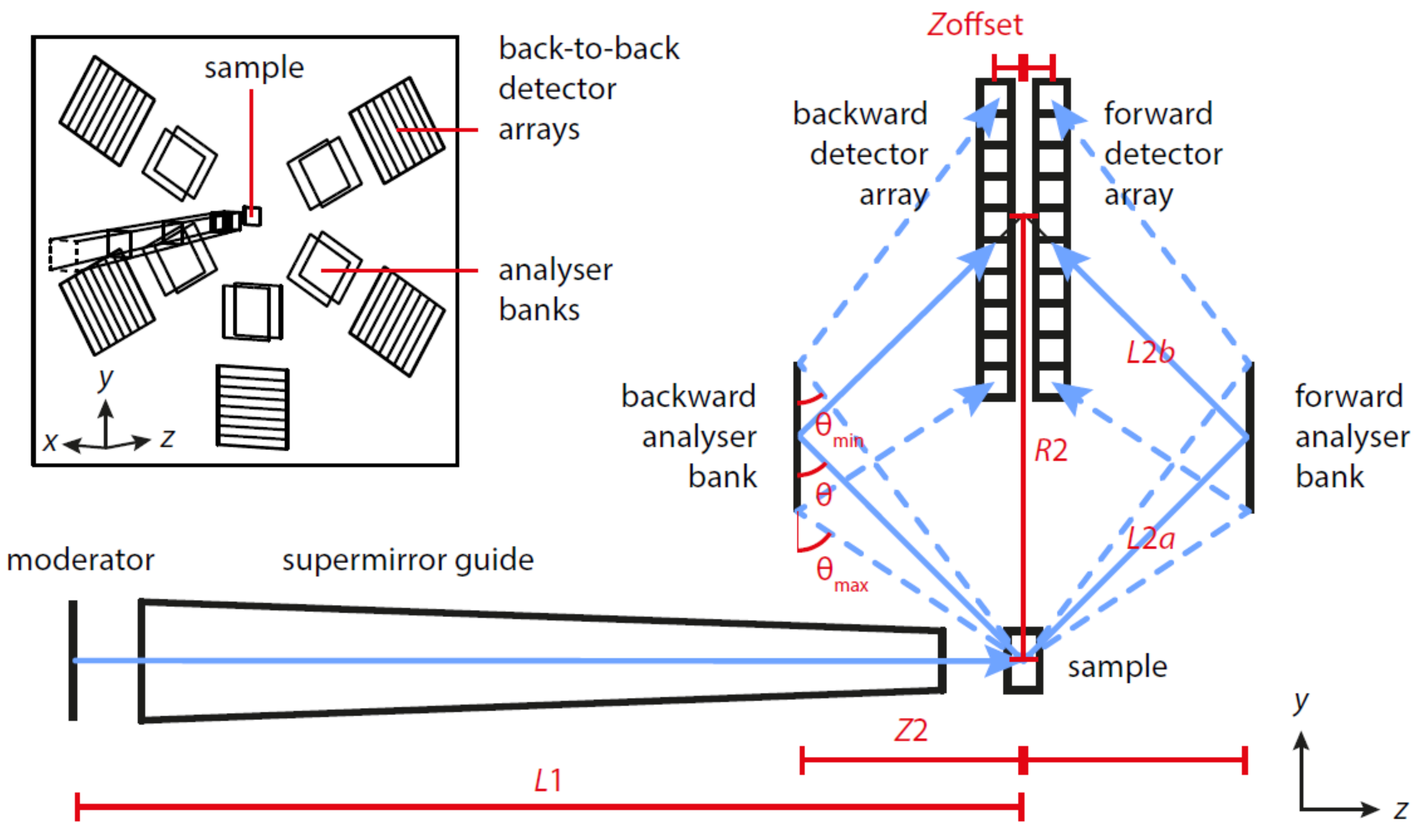




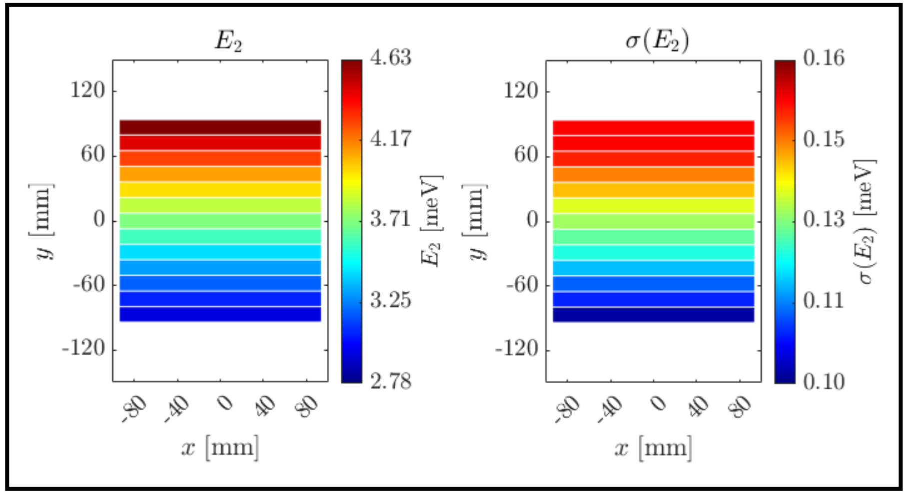


Focusing principles

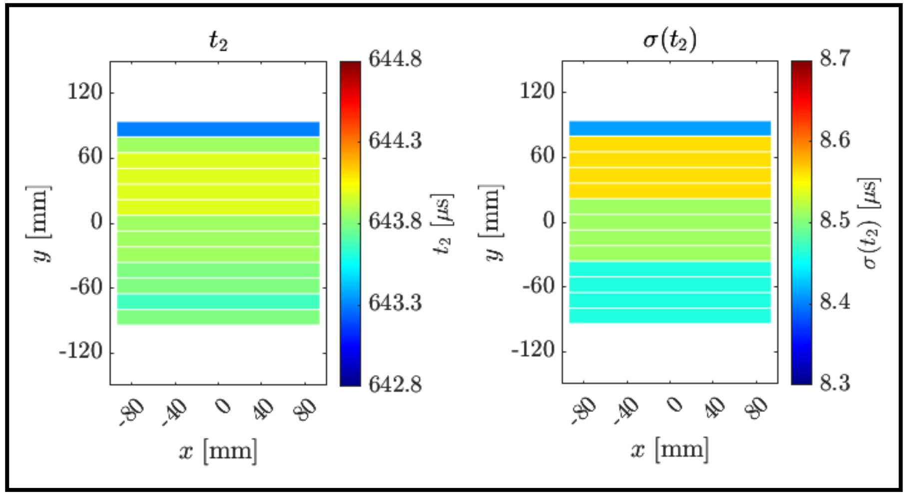
- Energy-focusing principle
- Time-focusing principle



Final energy (E_2) at detector



Secondary TOF (t_2) at detector



Key drivers & constraints

TOSCA+ to replace the entire secondary and achieve

1) At least 10-fold increase in detected intensity

- Increased solid angle, from 1 sr to >6 sr [×6]
- Better detector efficiency, from ~80% to ~90% [×1.1]
- Improved filter transmission, from 50% to >75% [×1.5]

2) Maximise SNR, aiming for 10-fold increase in SNR

- Beryllium filter thickness and blade spacing

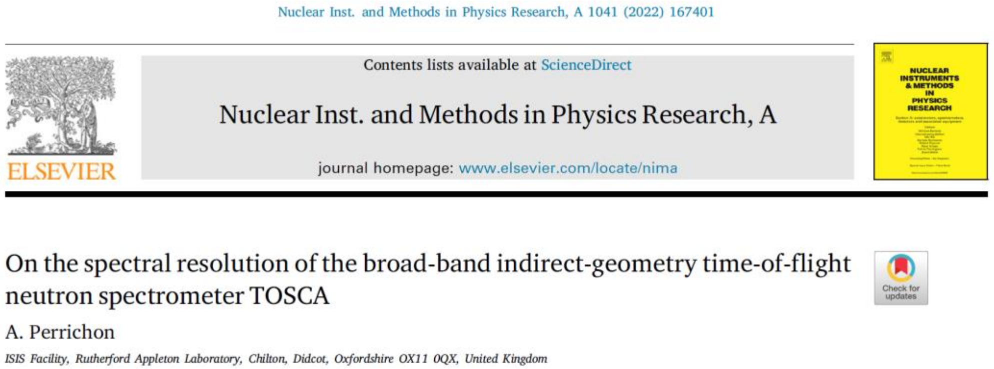
3) Match or improve the resolution, target of 1.2% of E_i

- Analyser design
- State-of-the-art detectors

Constraints

- Fixed sample position (no modification of the primary)
- Similar footprint
- Analyser lower and upper limits of the azimuthal angle: [27.5, 72]° (to fit diffraction bank, vacuum tube, cryostat)
- Entire secondary flight path in vacuum

Spectral resolution


Nuclear Inst. and Methods in Physics Research, A 1041 (2022) 167401

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Nuclear Inst. and Methods in Physics Research, A

journal homepage: www.elsevier.com/locate/nima

On the spectral resolution of the broad-band indirect-geometry time-of-flight neutron spectrometer TOSCA

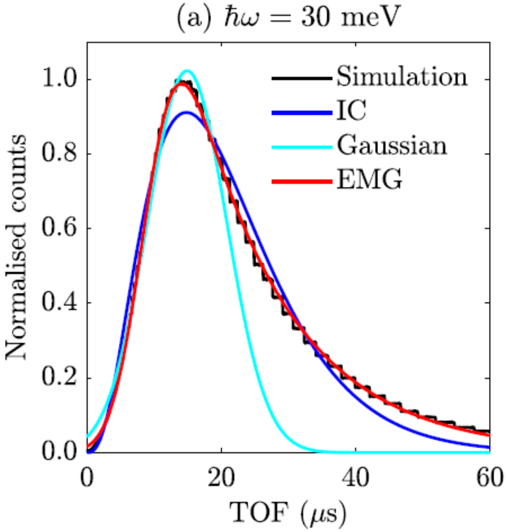
A. Perrichon

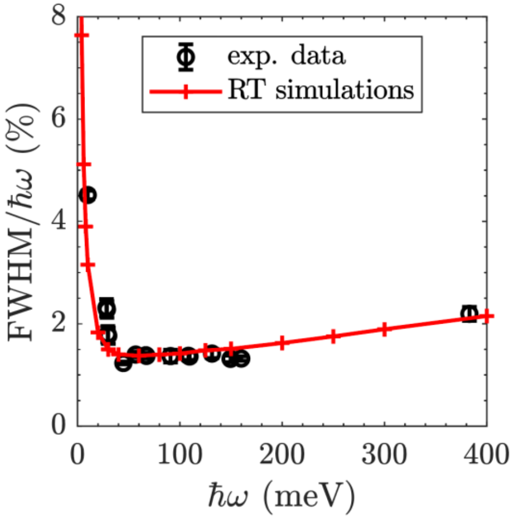
ISIS Facility, Rutherford Appleton Laboratory, Chilton, Didcot, Oxfordshire OX11 0QX, United Kingdom

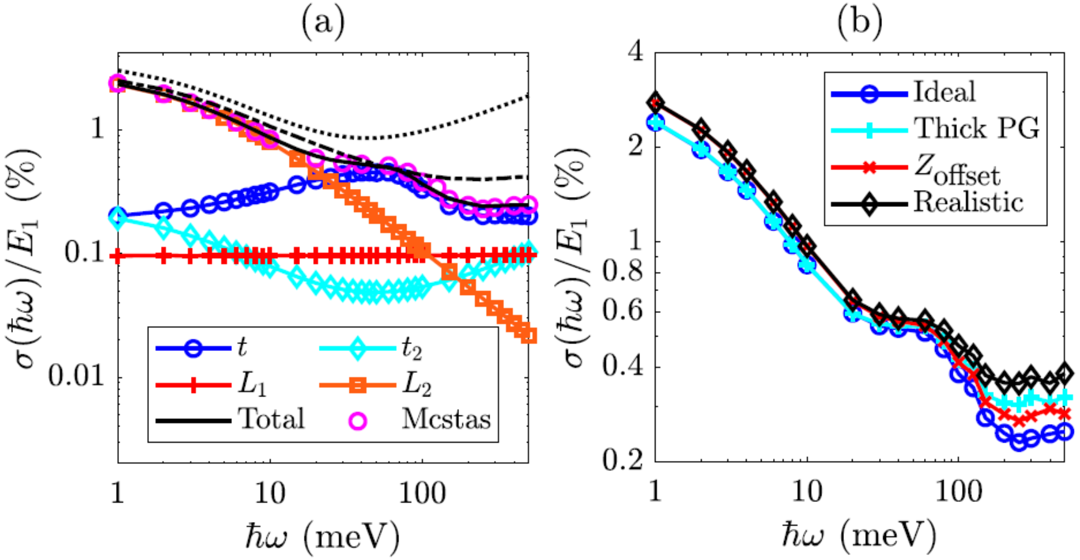
Mathematical model of the resolution that accounts for the TOF peak shape and component dimensions, and matches the experimental resolution and McStas simulations

To get the best possible resolution

- Design that minimises $V[t_2]$, then minimises $V[L_2]$
- Design that minimises Z_{offset}



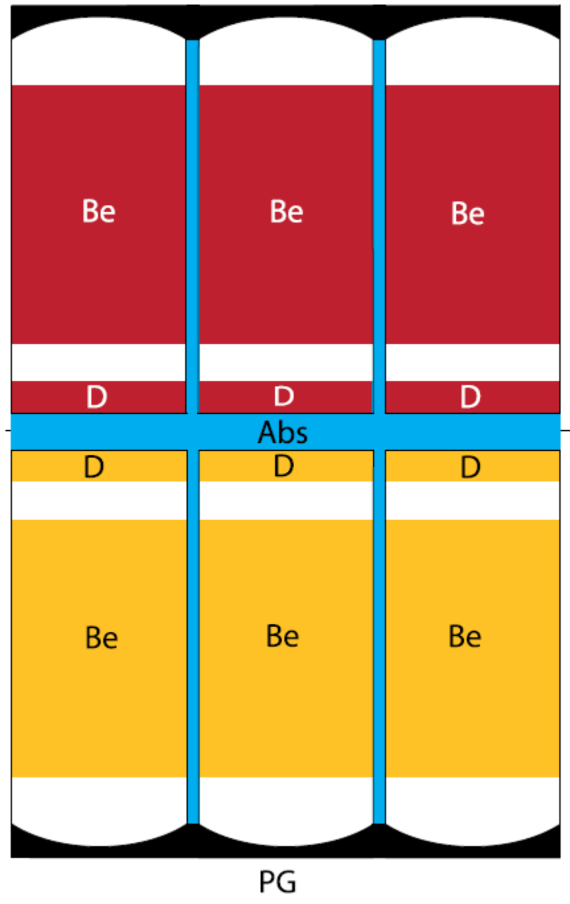




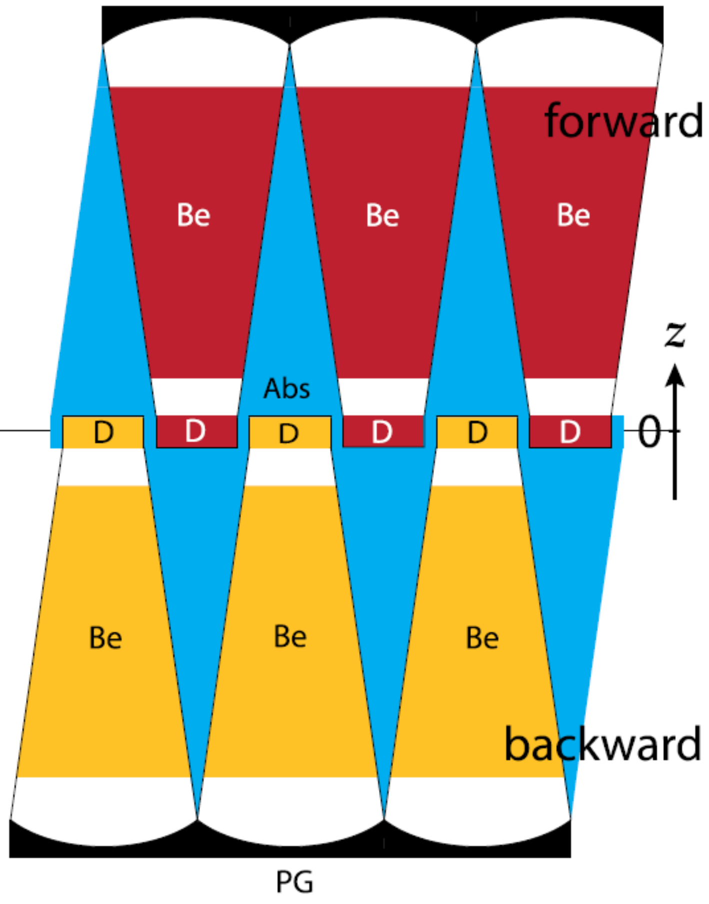
Assembly: spatial arrangement of analysers, filters and detectors

- Current TOSCA, VISION@SNS
- Mirrored forward and backward banks
- $Z_{offset} \geq 8$ mm, given by detector thickness and gap

Back-to-back assembly



Staggered assembly



- Staggered forward and backward banks
- Z_{offset} <3 mm, possibly 0
- Fewer detectors, less Be from horizontal focusing
- More room for Be filter, better SNR

HOPG tiling strategy

Orthogonal tiling (back-to-back)

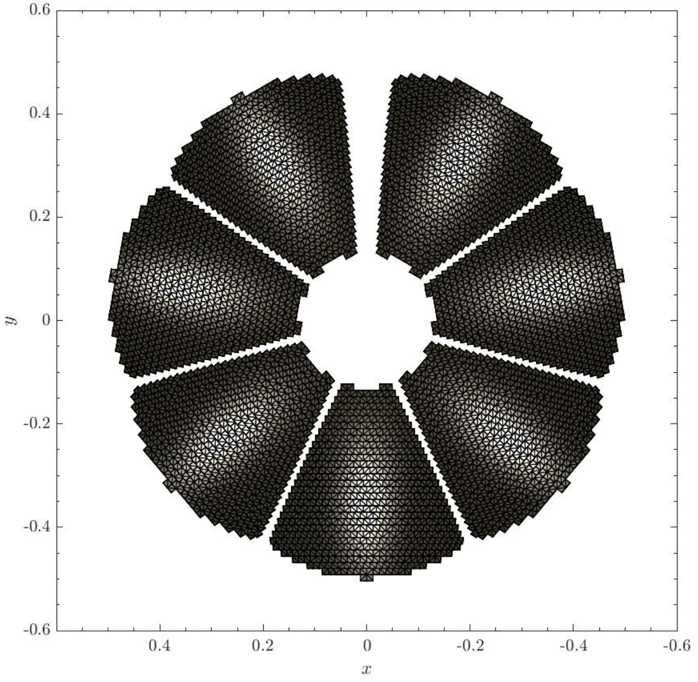
- Vertically focusing
- Horizontally focusing
- Max 6.6 sr (14 arms)
- Min 1.3% E_i

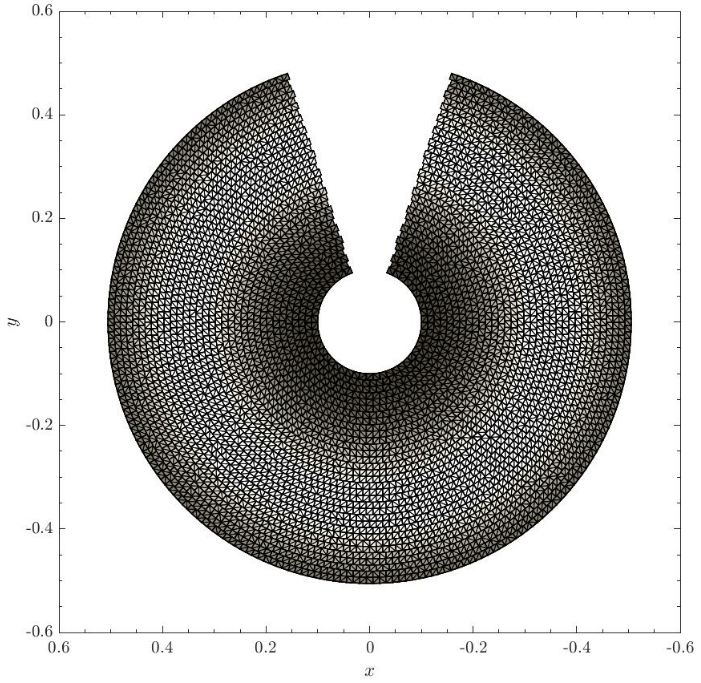
Radial tiling (back-to-back)

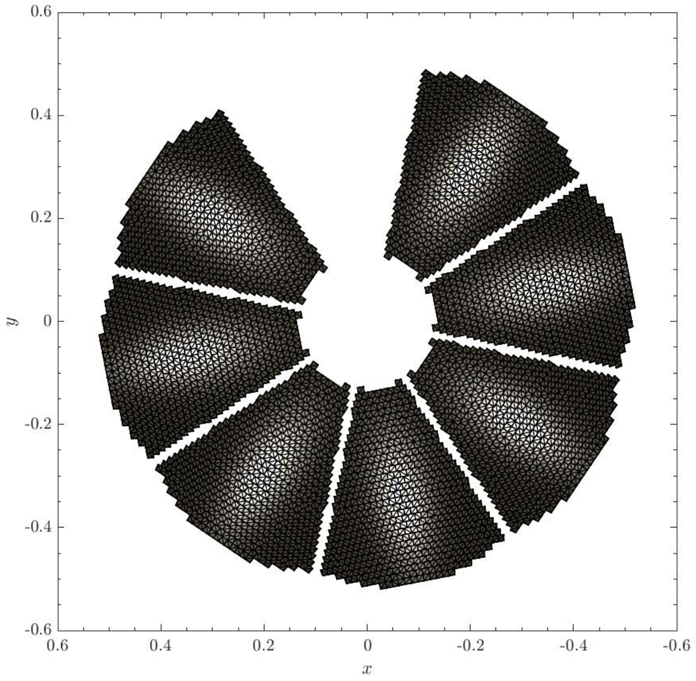
- Vertically focusing
- Horizontally flat
- Max 6.1 sr (2 continuous arms)
- Min 0.9% E_i

Orthogonal tiling (staggered)

- Vertically focusing
- Horizontally focusing
- Max 6.3 sr (14 arms)
- Min 1.0% E_i







Design process: Choice of the assembly

Evaluation of the assemblies: performance, feasibility, cost

Increasing the number of arms

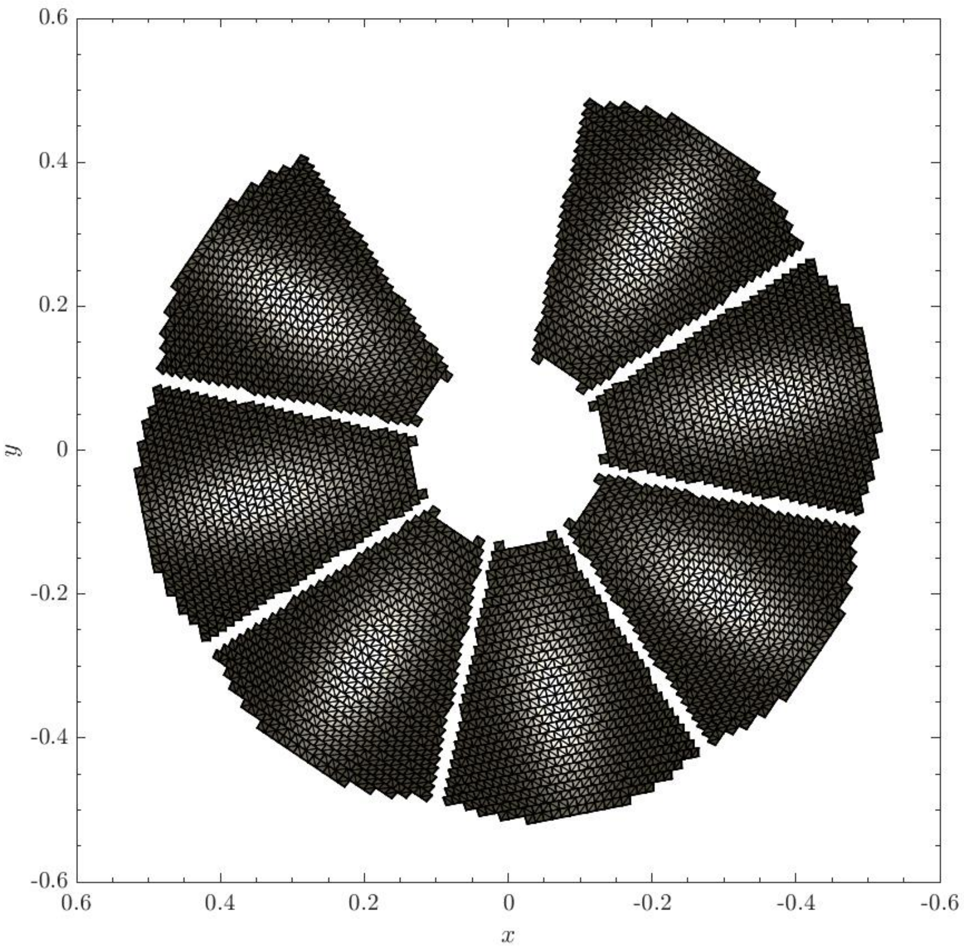
- Improves the resolution (less blur)
- Decreases the solid angle coverage
- Increases the cost

Staggered over back-to-back assembly, at equal solid angle

- Better resolution (lower Z_{offset}, worst blur)
- Better SNR (longer Be filter)
- Significantly cheaper
- Complex geometry

Selected assembly is <u>staggered with 14 arms</u>

- Maximum gain for a resolution of 1% E_i
- Best possible SNR



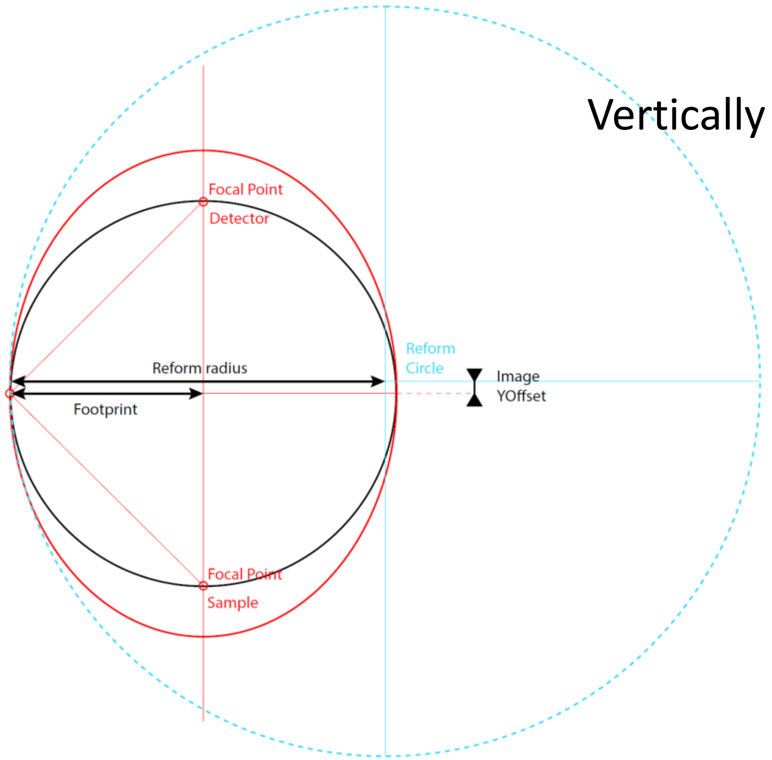
Staggered 14 arms, double focusing

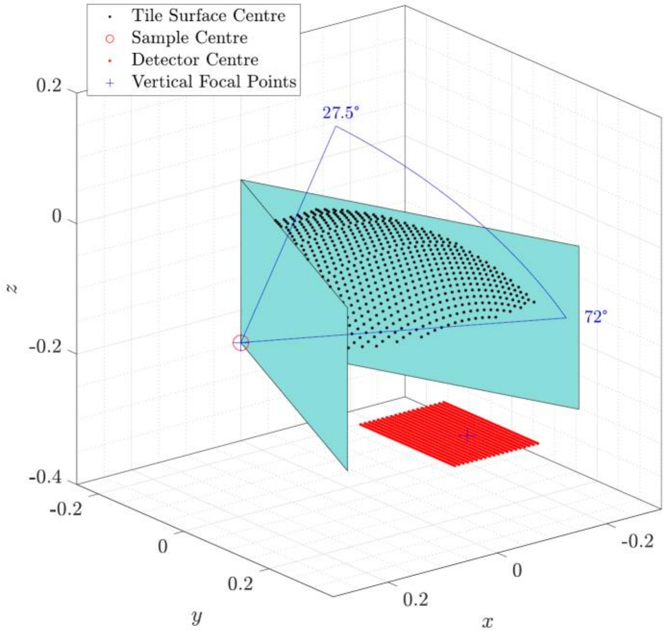
Ten parameters to fully describe the analyser
Tiles located on a 3*d* ellipsoid (6 free parameters)
Tiles tilted to face a distant focusing point (2 free parameters)

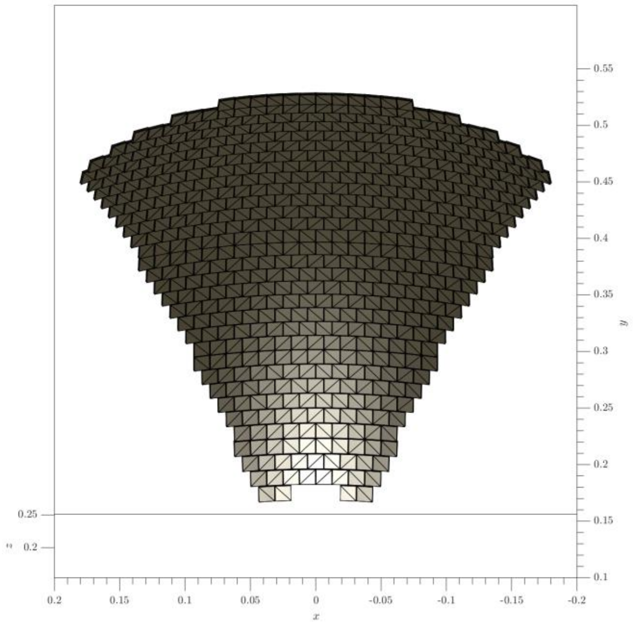
Spatial constraints:

- Polar coverage (45°)
- Azimuthal coverage (27.5-72°)
- Tile dimensions (12-by-12 mm, 2 mm thick)
- Spacing between tiles (0.5 mm)
- Gap to border (6 mm)

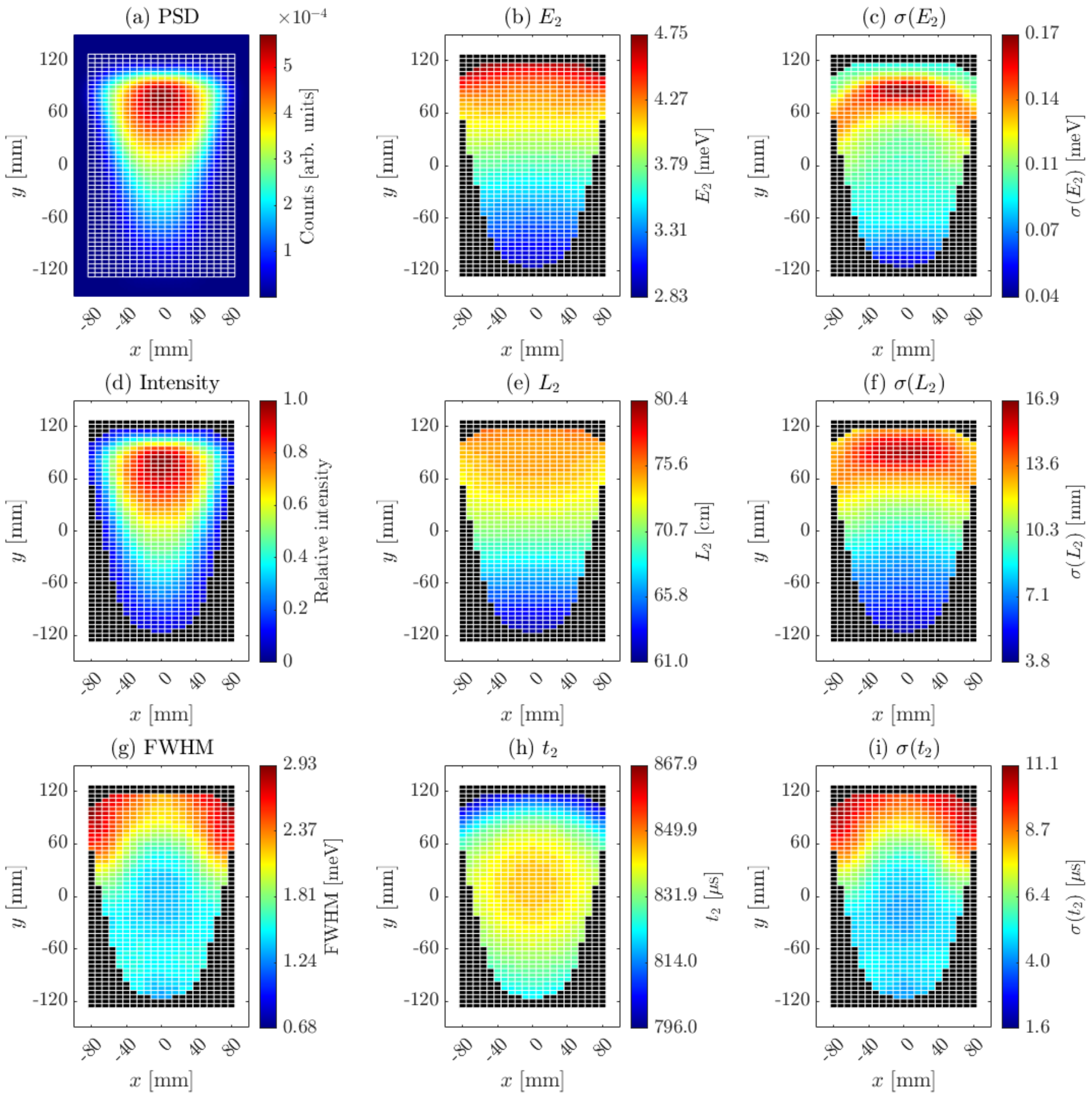
Per arm: 596 tiles; Total: ~8400 tiles ~1.2 m^2





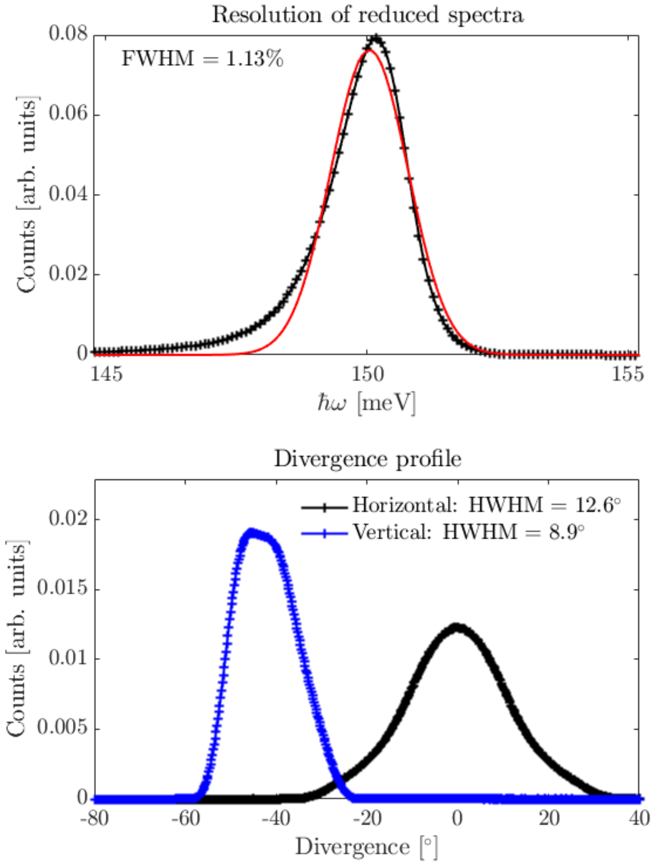


Proposed design: Profile at detector



Staggered 7 arms, double focusing (596 tiles)

Gain from solid angle: 6.43 (6.12×1.05)
Gain from detector efficiency: 1.10
Total gain: 7.07



Design process: Detector system

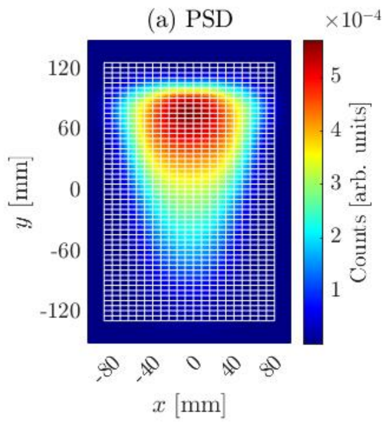
Requirements

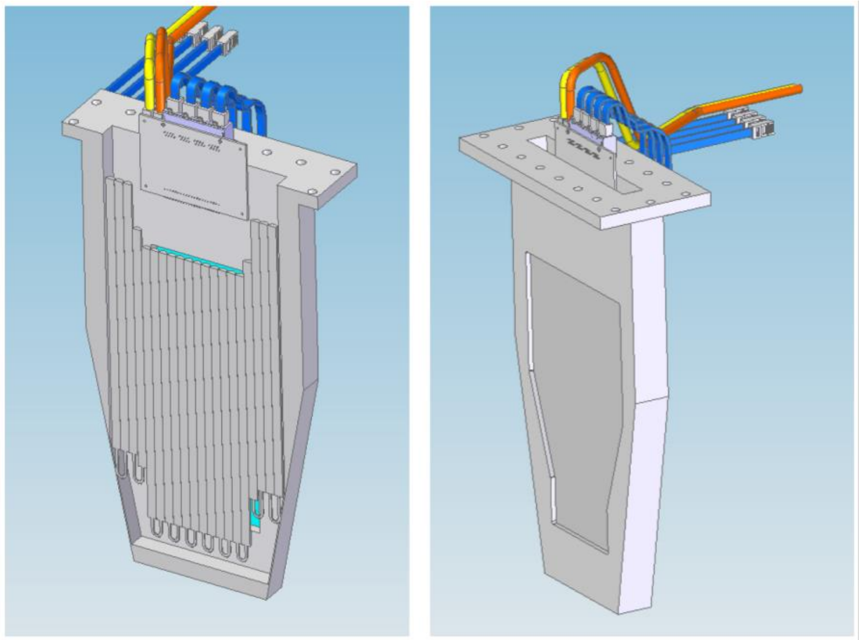
- Efficiency >90%
- Spatial resolution 5—8 mm
- As thin as possible (*z* = 0 position)
- Variance in time as low as possible (capture + resolution)

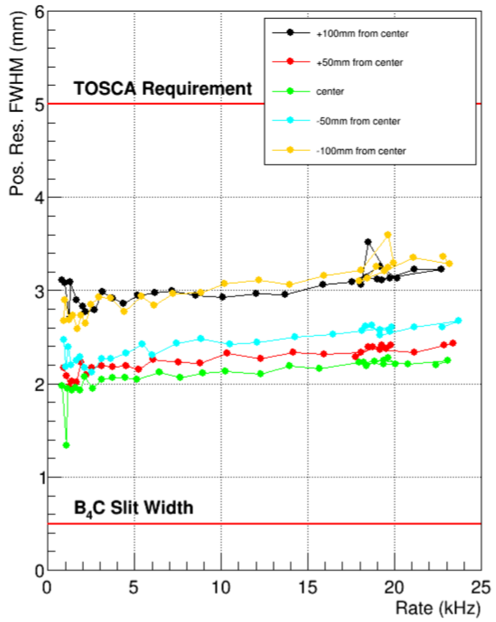
➢ Technology: <u>High pressure 3He PSD cylindrical tubes</u>

Optimal solution

- PSD tubes with ∅ 8 mm and length 25 cm
- 20 tubes in series of 4
- Single row, stacked vertically
- 20 bar pressure, 89% efficiency
- Est. std of 2 μs from capture + 1 μs resolution







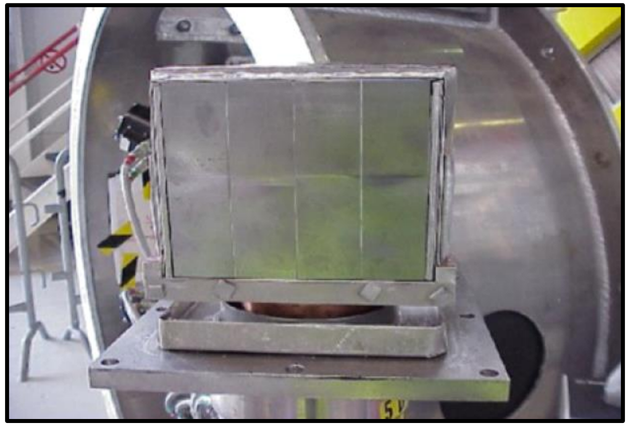
❖ Ongoing characterisation by Davide Raspino, ISIS Detector group

Design process: Beryllium filter

Be filter

- Assembly of beryllium wedges & neutron absorbing blades

- Suppresses high-energy neutrons
- Suppresses stray neutrons
- Transmits analysed neutrons

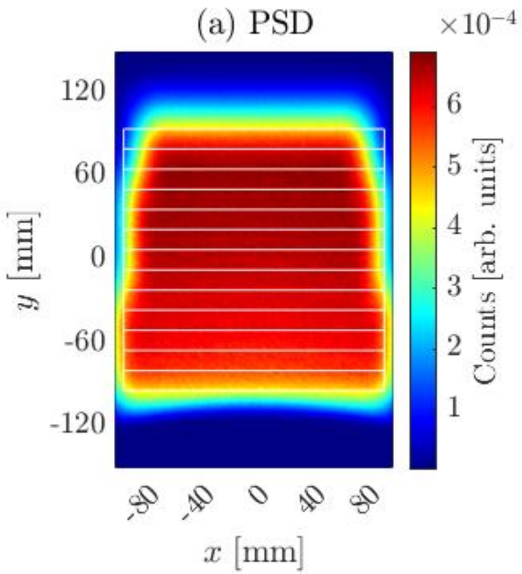


Current filter

How to simulate the built-in collimation?

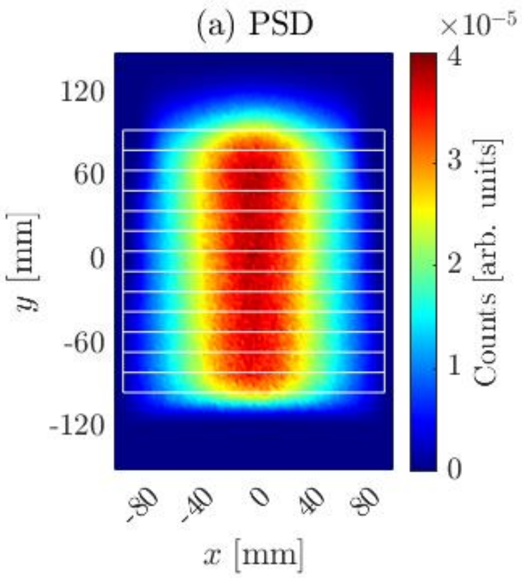
Analytically; triangular transmission with 14° divergence cut-off
Geometrically; intercept check between blades and neutron trajectories

No collimation



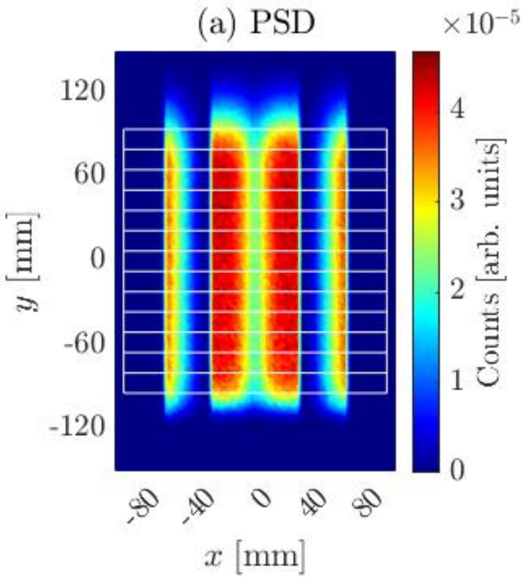
Transmission 100%

Analytical collimation



Transmission 56%

Geometric collimation



Transmission 48% (44%)

Design process: Beryllium filter

How to simulate the beryllium itself?

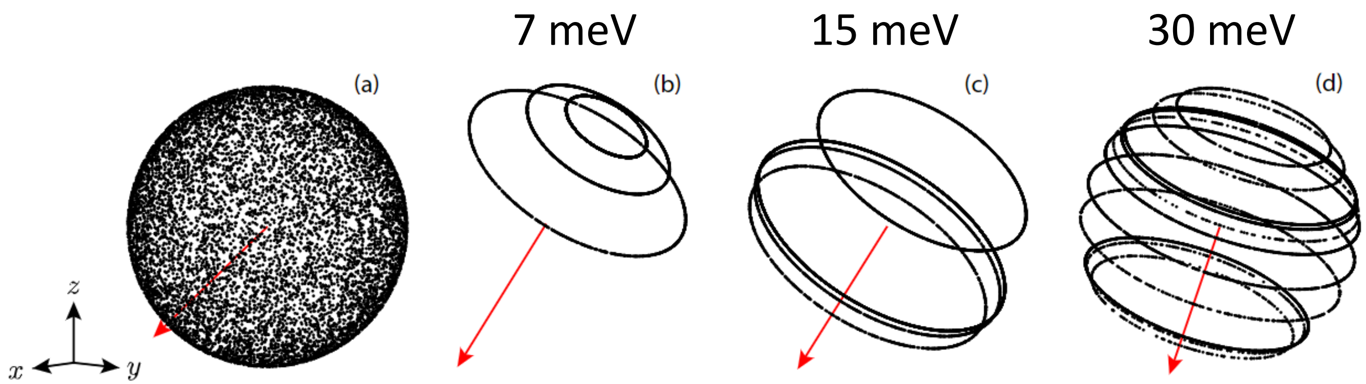
- Isotropic coherent scattering *or* (energy-dependent) Bragg scattering
- Isotropic incoherent scattering
- Absorption

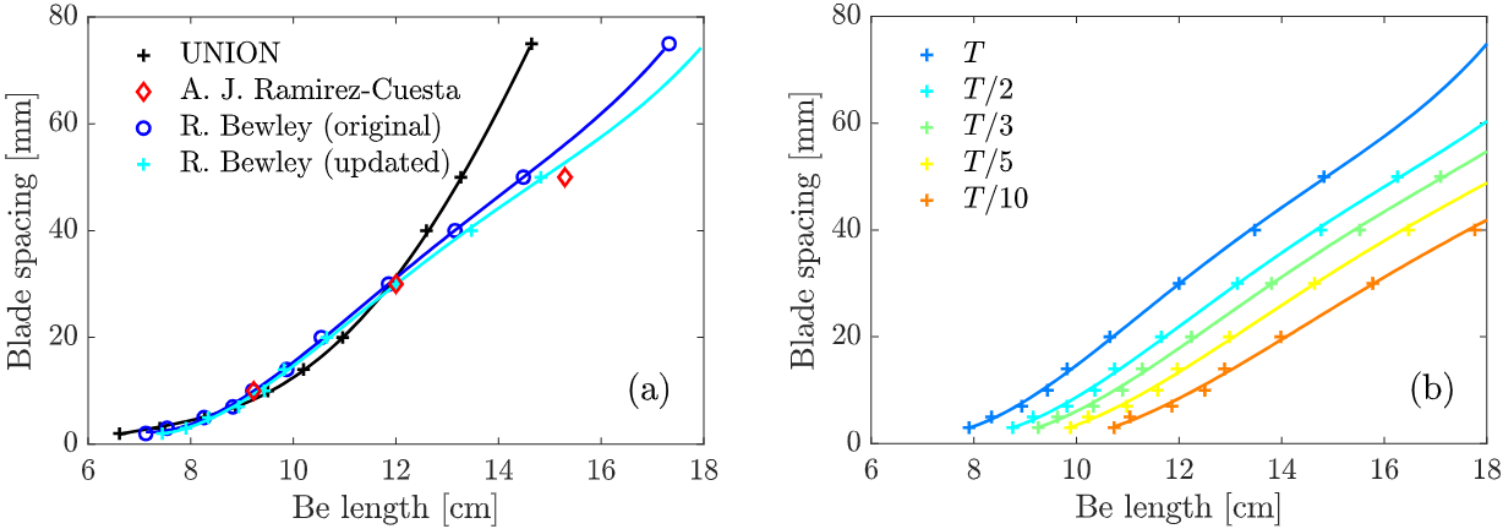
➢ Large variations in absolute transmission values depending on the scattering kernel

➢ Relative variations in transmission similar in all codes

Which spacing to choose for a given Be length?

- Iso-transmission relations

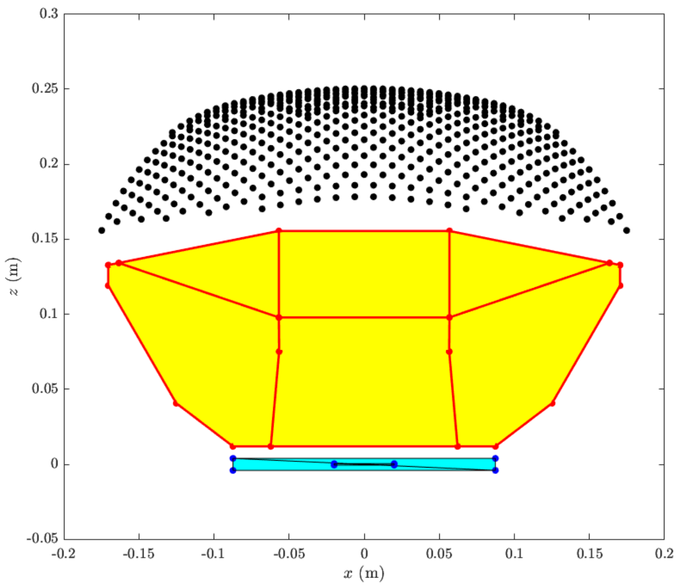


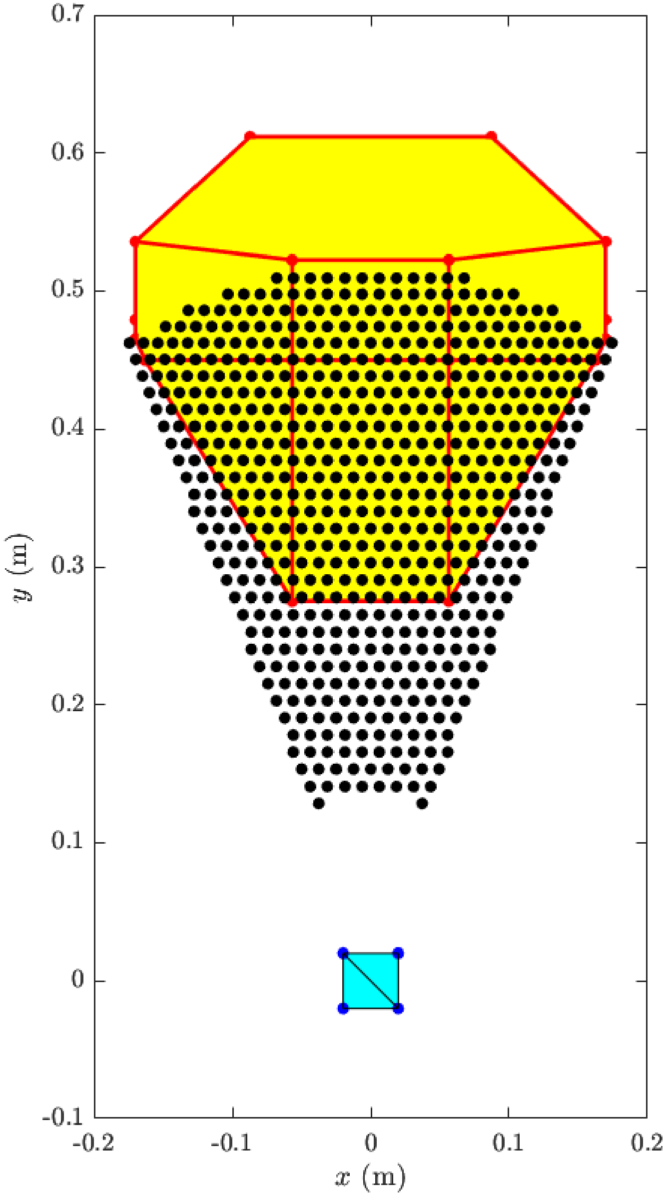


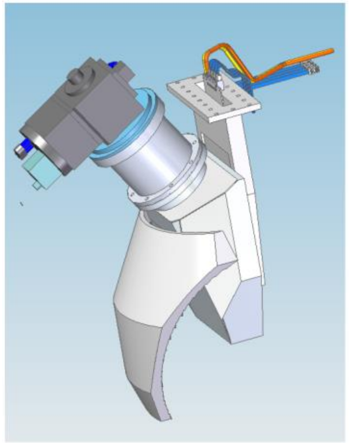
Be filter dimensions

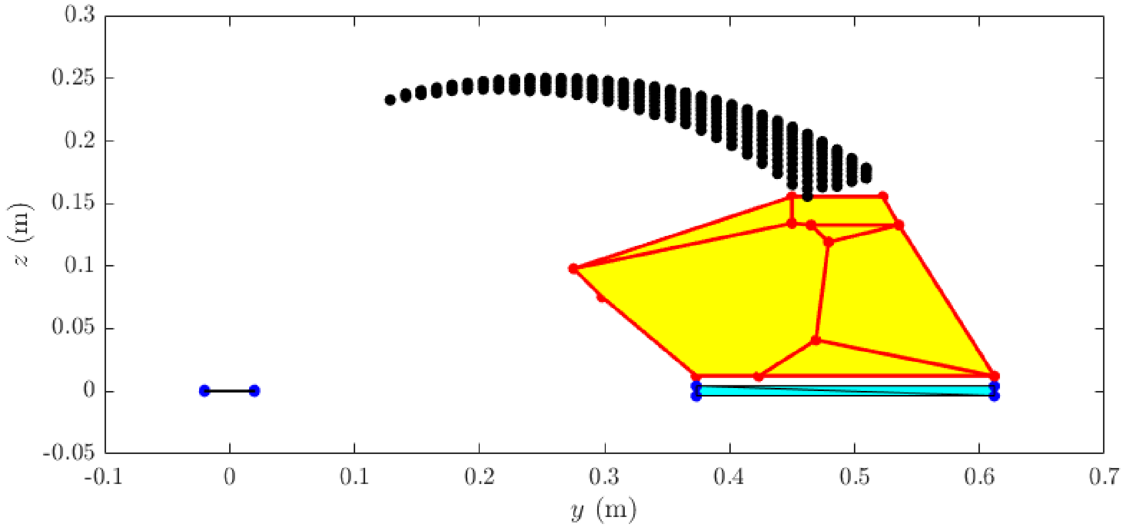
Envelope max. dimensions

- Line-of-sight
- Gap between filter and detector
- Adjacent filters
- Image shape and dimensions
- *Frame design & engineering requirements*



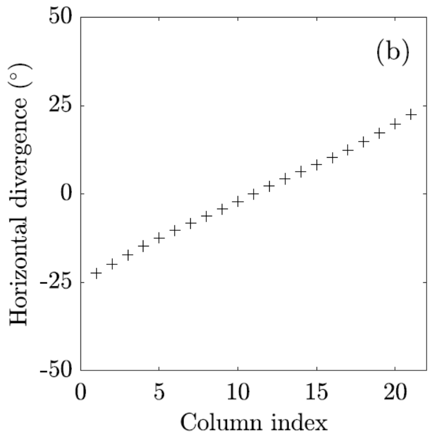


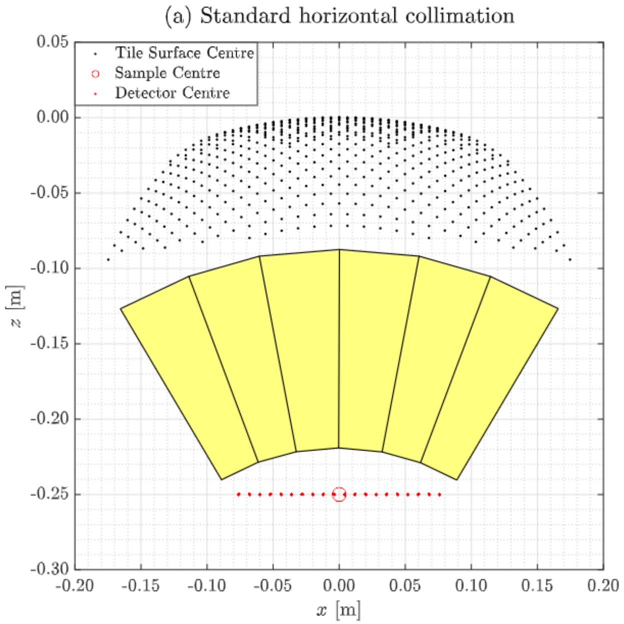


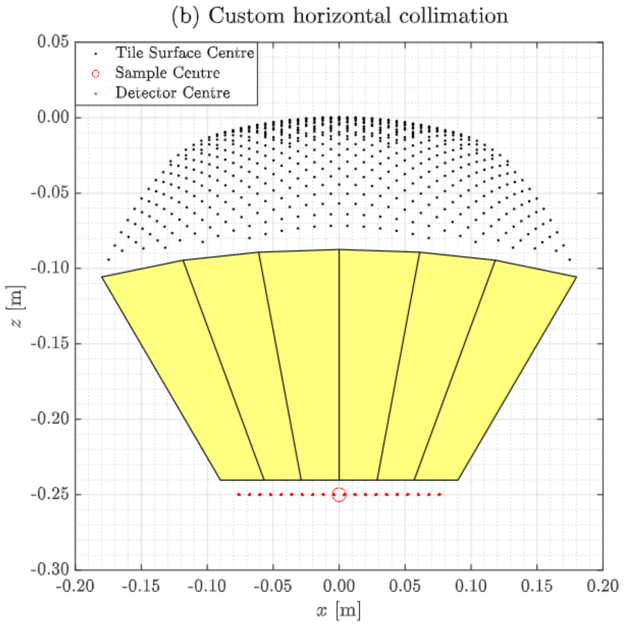


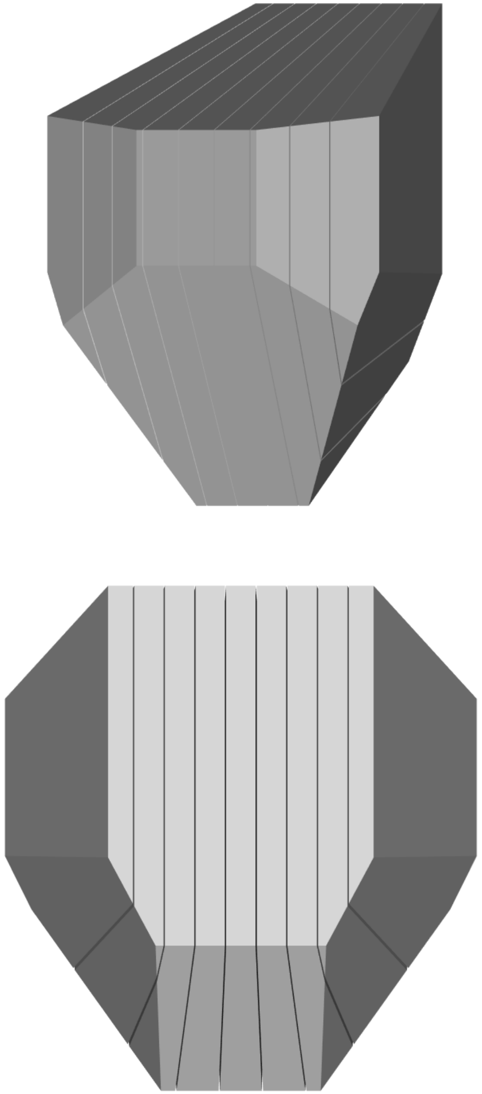
Design based on divergence profile

Option A
Horizontal
collimation









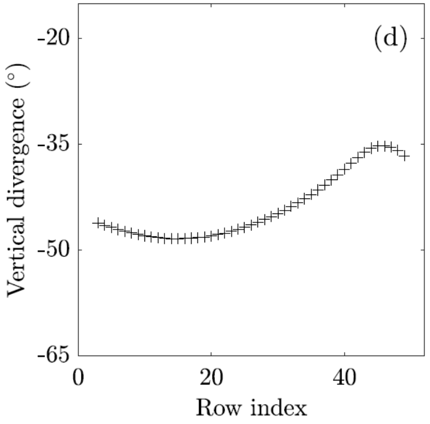
Standard radial collimator
- ✓ Easier to manufacture
- × Shorter path

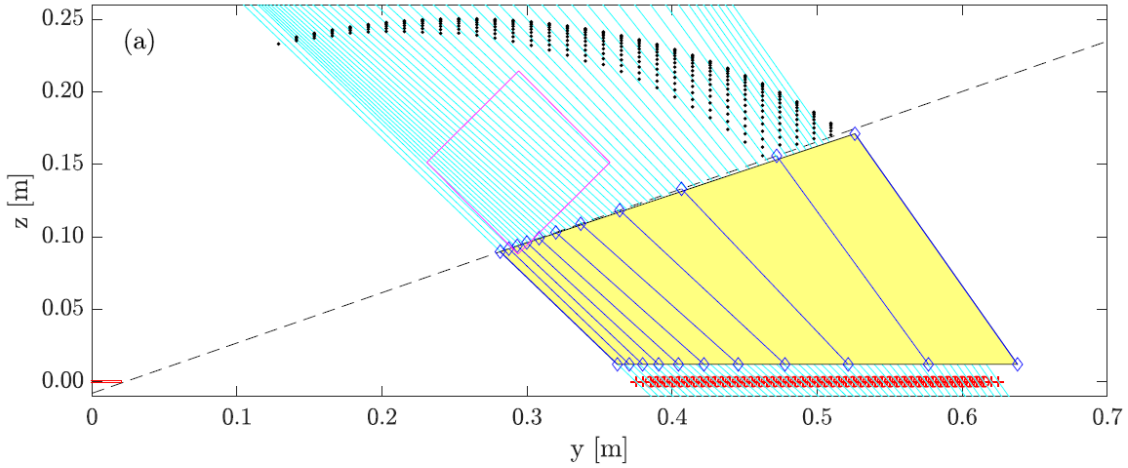
Custom radial collimator
- × Complex to manufacture
- ✓ Maximum path

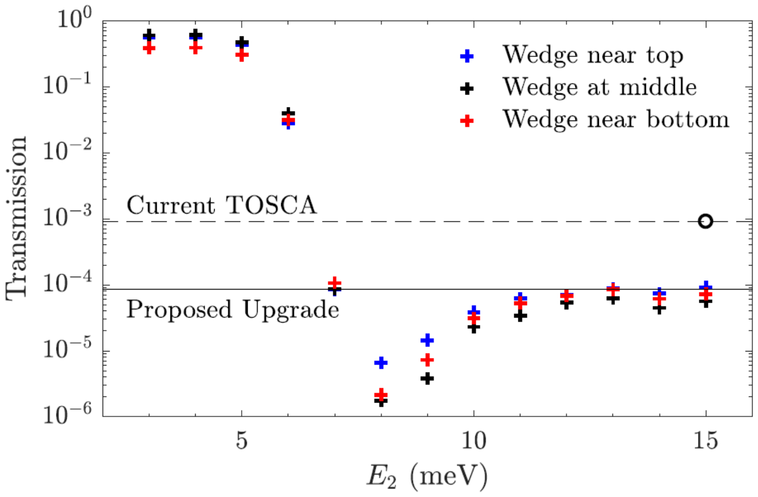
- × Performance vary with height
- × Challenging to clamp
- × Direct path for parasitic scattering from Al windows

Design based on divergence profile

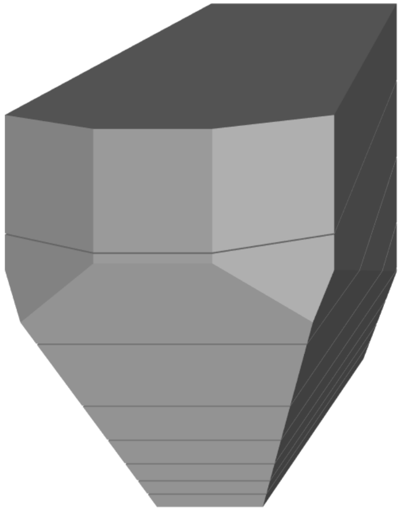
Option B
Vertical
collimation

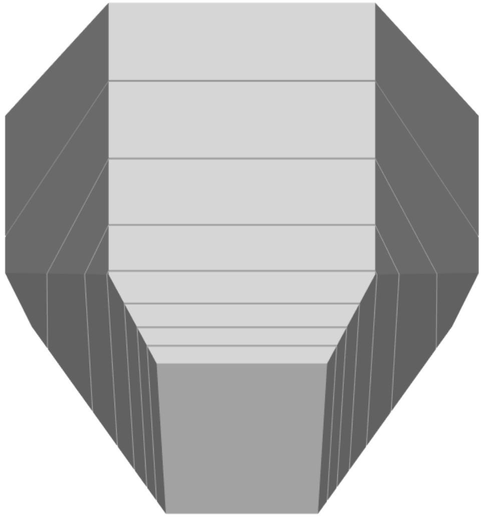




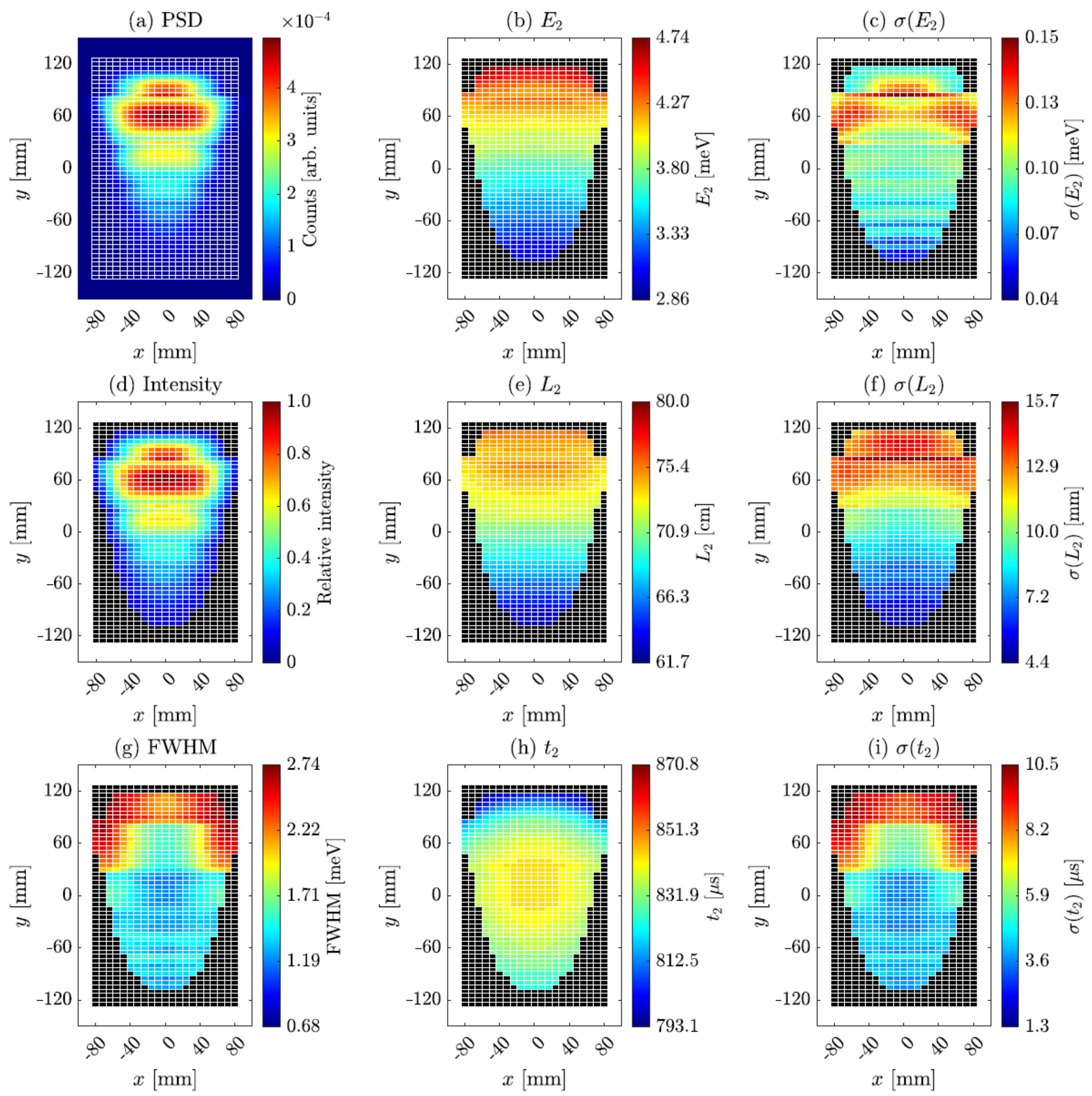


- Complex but feasible
- ✓ Maximum path
- ✓ Uniform performance
- ✓ Easier to clamp
- ✓ Limits background from Al window scattering





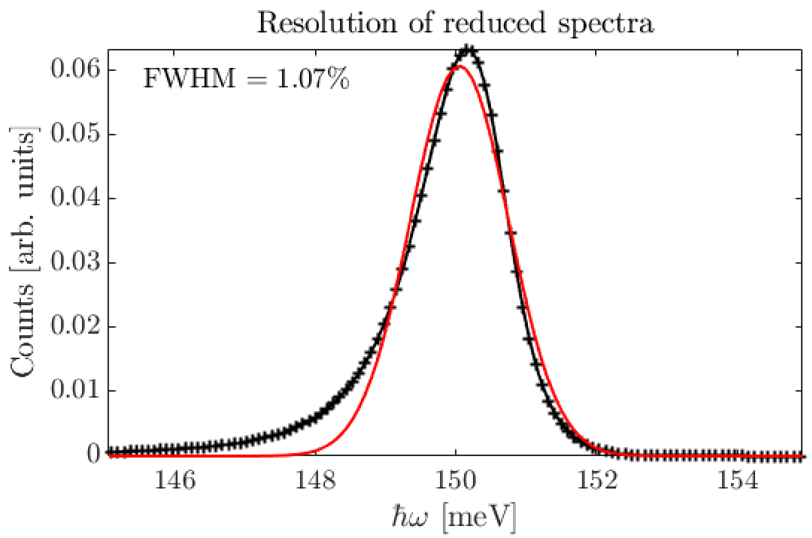
Proposed design: Profile at detector



Performance of the entire secondary

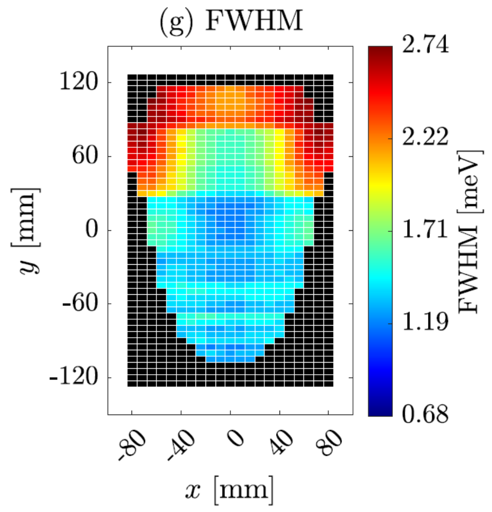
Gain from solid angle: 6.43
Gain from detector efficiency: 1.10
Gain from filter efficiency: 1.63 (78% transmission)
Total gain: 11.52

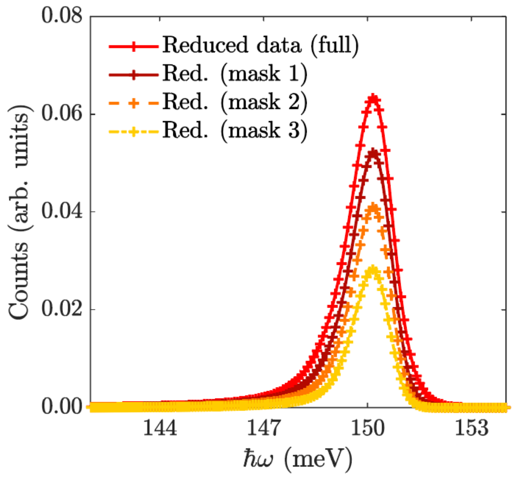
Average resolution 1.07%

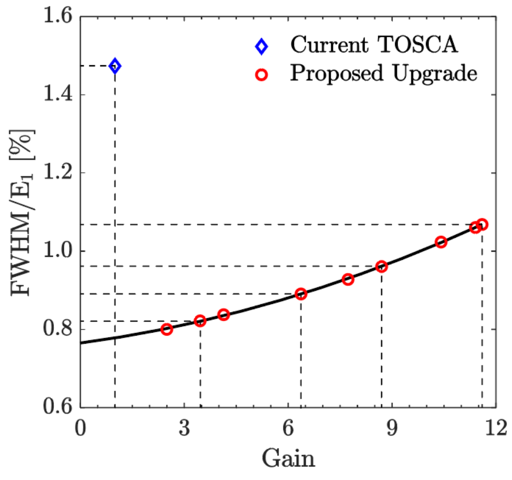


Flexible resolution

- Trade-off gain/resolution using masks in the data reduction
- ➢ <1% resolution for high resolution experiments, line width measurements

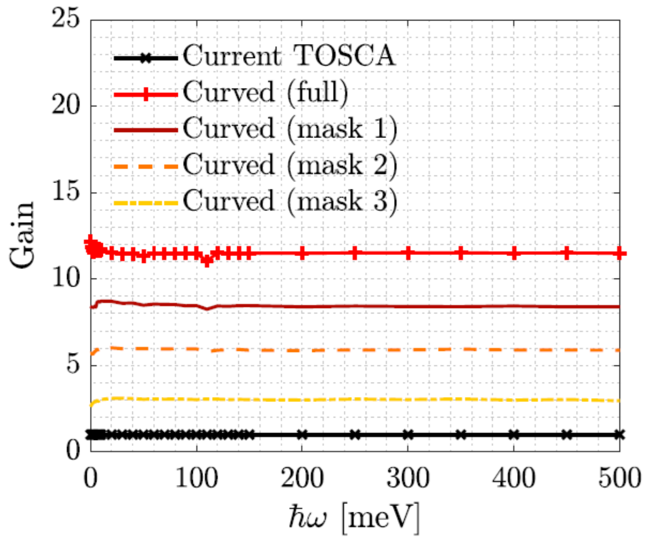


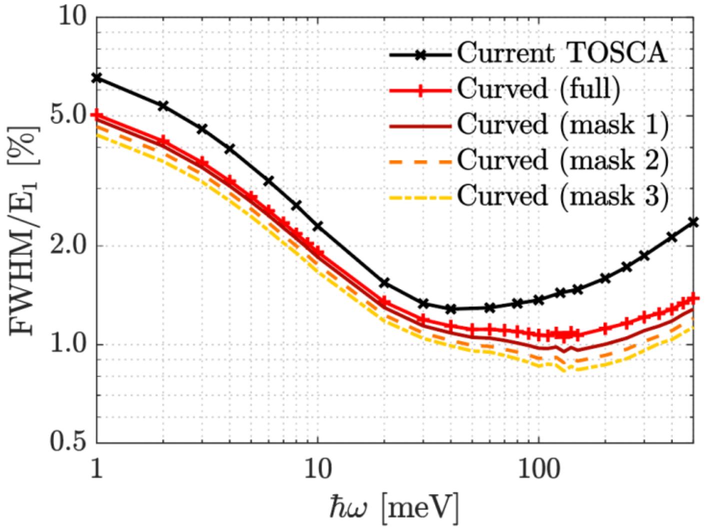




Energy-dependence of the gain and spectral resolution

- Gain factor 10+
- Overall improvement of the resolution
- Improved SNR





TOSCA+ secondary spectrometer

- Staggered assembly of analyser modules & vertically-collimated Be filters to push the limits in **solid angle coverage** and **SNR**
- Analyser design to spread "image" on detector to improve **energy resolution** & allow flexible **gain/resolution trade-off** in the data reduction

Compared to other NVS instruments

- Best resolution worldwide in standard operation mode, for a large sample (40×40 mm^2 flat cell)
- Very large solid angle, very high SNR
- Competitive with existing and future instruments

Instrument	Solid angle (sr)	Resolution (% E_i)
TOSCA	1	1.5
IN1 Lagrange	2.5	2-3 (Cu220), 1.5-2 (Cu331)
VISION	3.6	1.5
VESPA	5.3	2.0 (LR), 0.8 (HR)
TOSCA+	6.3	1.1 (0.8)

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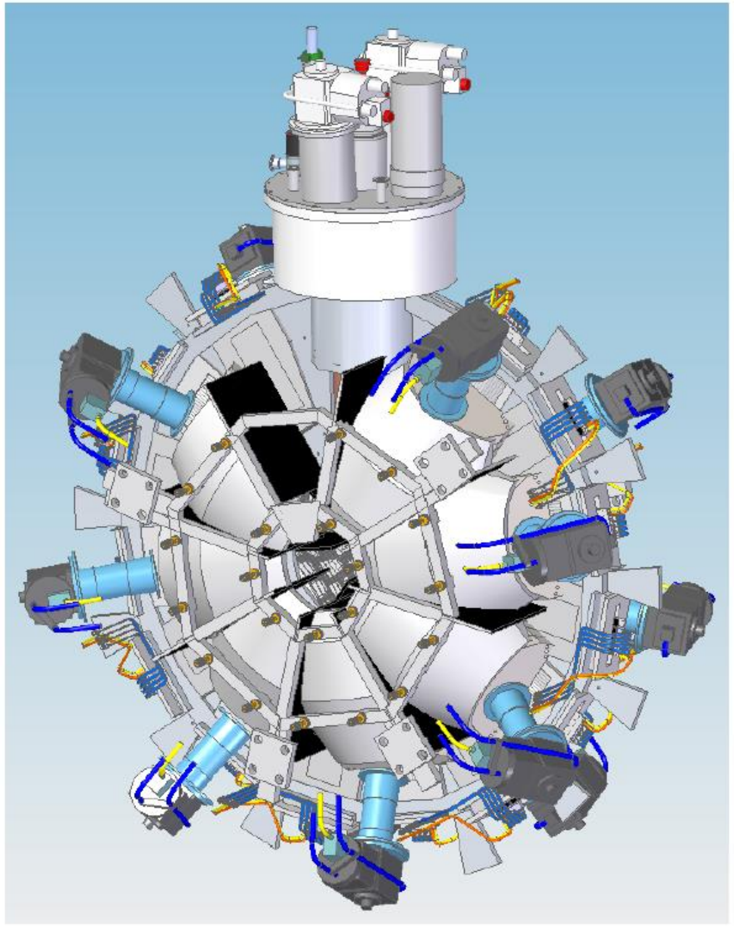

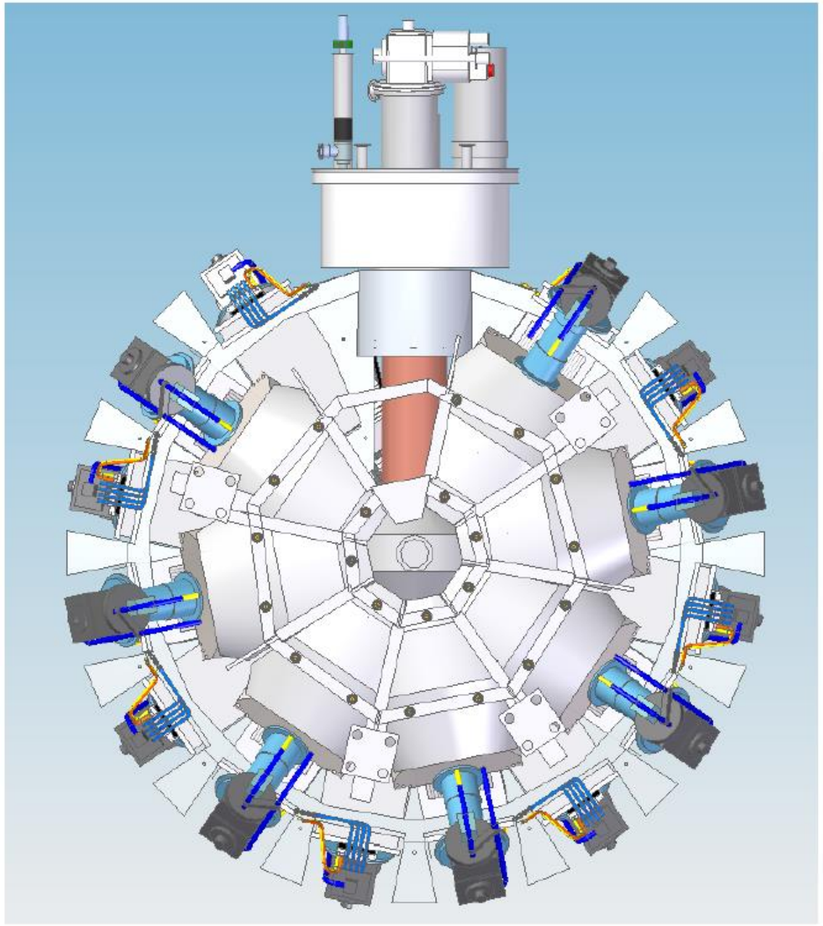

Thank you for your attention!