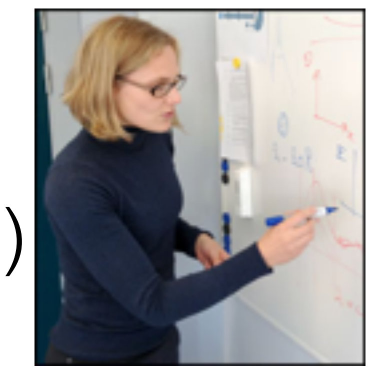
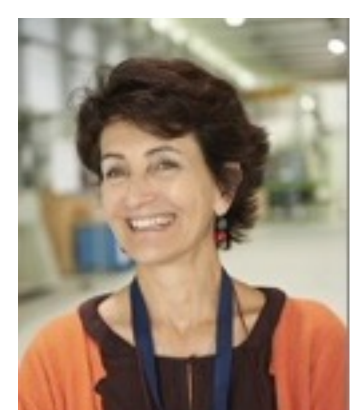
C-Spec

C-Spec: The cold chopper spectrometer of the ESS



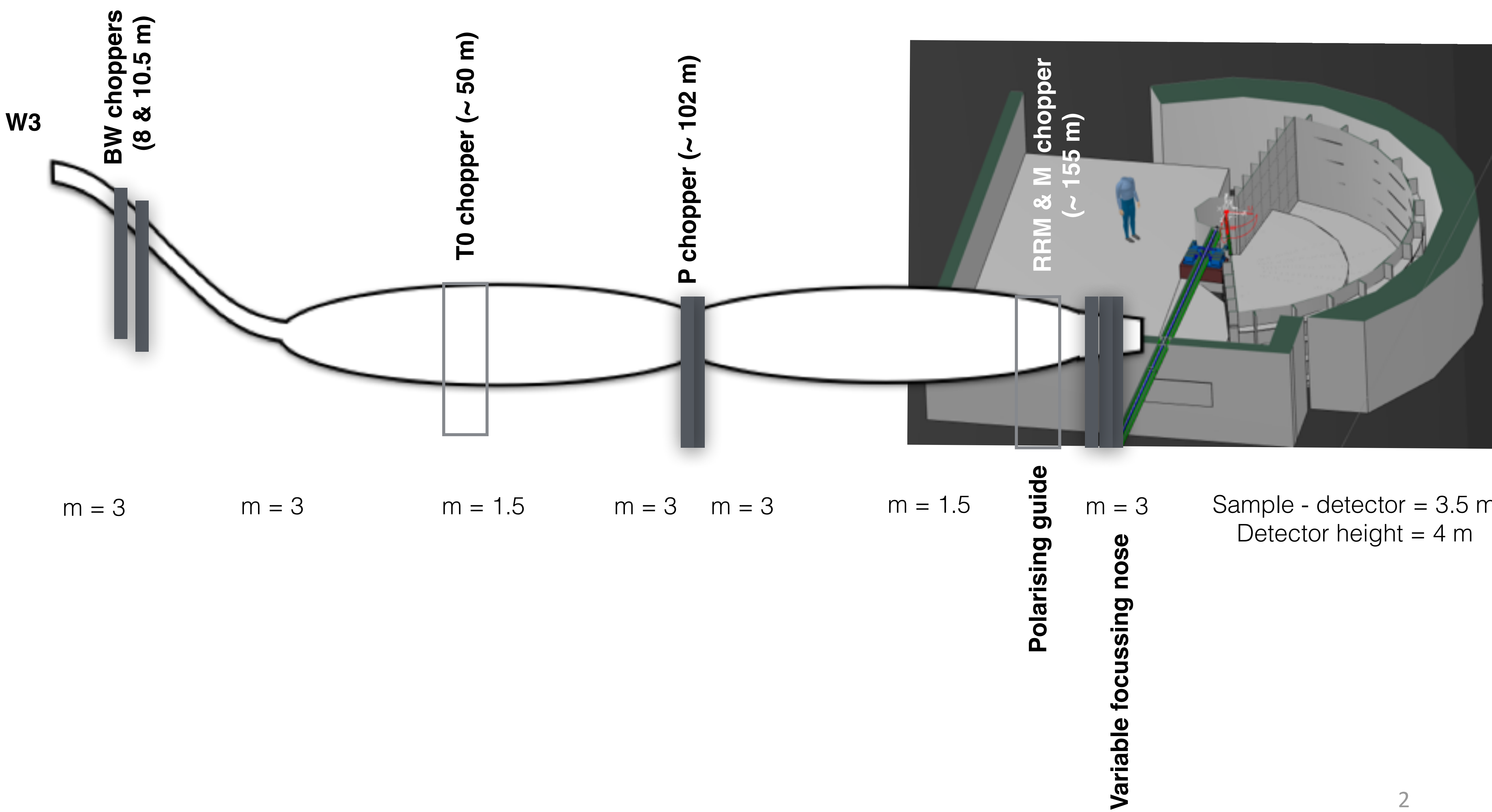
Lead Scientist: P.P. Deen (TUM)
Lead Engineer: Joseph Guyon le Bouffy (LLB)

TUM: W. Lohstroh, J. Neuhaus, W. Petry
LLB: S. Longeville, C. Alba-Simionesco



C-Spec

An overview



CSPEC high level requirements:

1. **Wavelength range = 2 – 20 Å.**
2. CSPEC shall probe excitations up from 0.005 up to 20 meV.
3. CSPEC shall measure in repetition rate multiplication configuration.
4. **CSPEC shall be capable of energy resolutions down to ΔE/E = 1% at the highest wavelengths.**
5. CSPEC shall be capable of spatial resolution ΔQ/Q = 2%.
6. **CSPEC shall provide a signal to noise of 10^4 at 5 Å. Signal to noise is defined as the peak intensity of the elastic line of a vanadium sample versus background obtained far away at a time of flight when the background level has been reached.**
7. The chopper cascade shall ensure that each incident wavelength arrives when the scattering from the previous incident wavelength has reached background levels.
8. **The neutron beam at the sample position shall illuminate a sample area ranging from 4 x 2 cm^2 to 0.5 x 0.5 cm^2.**
9. **CSPEC should follow kinetic processes with time steps of one minute.**
10. The detectors will ensure the Q and E requirements (including ΔE and ΔQ) outlined in the CSPEC proposal.
11. **CSPEC shall probe magnetic excitations in magnetic fields up to 12 T.**
12. **CSPEC shall ensure the possibility to perform polarisation analysis in the future.**
13. The systems design shall provide the space and flexibility necessary to host and drive future developments.
14. **Sample environment for the wide range of scientific cases studied on CSPEC must be consistent with the demands of signal to noise.**

C-Spec

Grand challenges & CSPEC Science case:

Energy: Solar cells, batteries, thermoelectric materials, hydrogen storage

Climate: CO_2 capture and storage (carbon nanotubes) Low carbon technologies in cement, steel and chemical industries

Health: Drug delivery, proteins dynamics and behaviour, hydrogen bonding, quantum effects in the origin of life

Digital Society: Magnetic storage and reading, Spin liquids, novel magnetic behaviour (Topology!)

C-Spec

1st Day experiments

J. Pieper, Tartu University

Time dependent laser pump probe studies of proteins.

Structure–dynamics–function relationship at the atomic level. To date only studies in steady state experiments with variation of external parameters temperature and hydration.

a) light harvesting and excitation energy transfer in the photosynthetic antenna complex LHC II

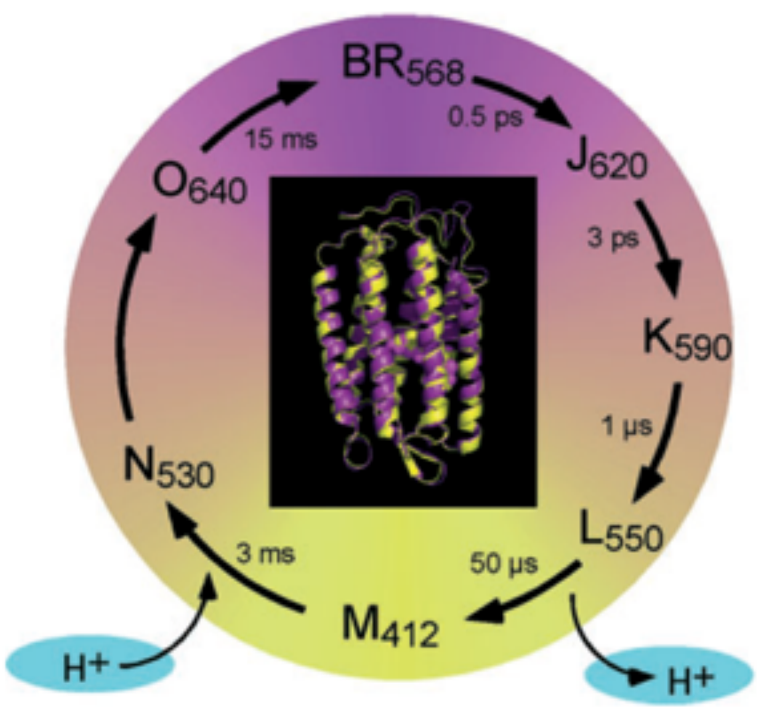
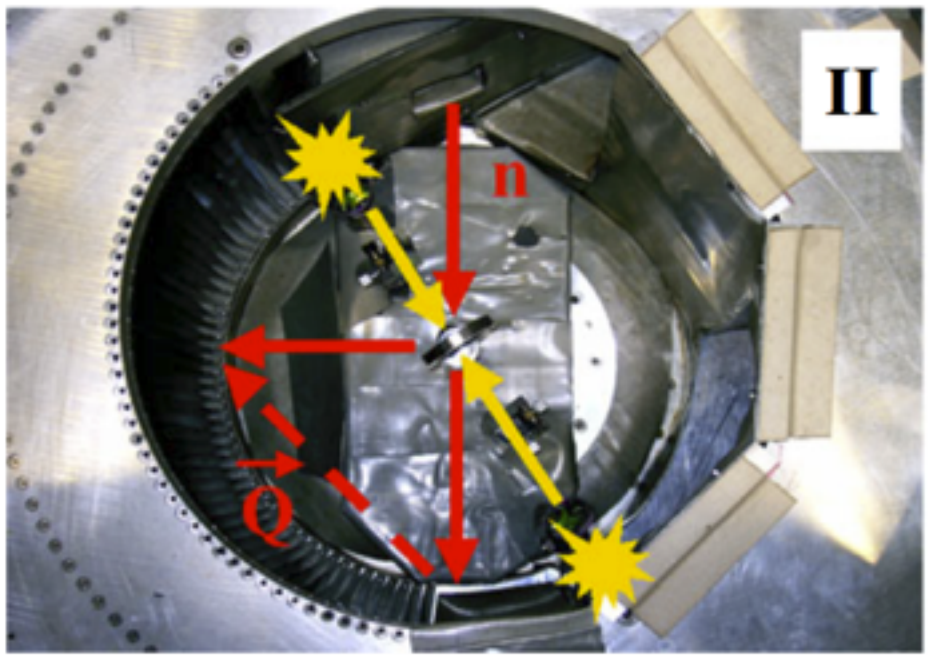


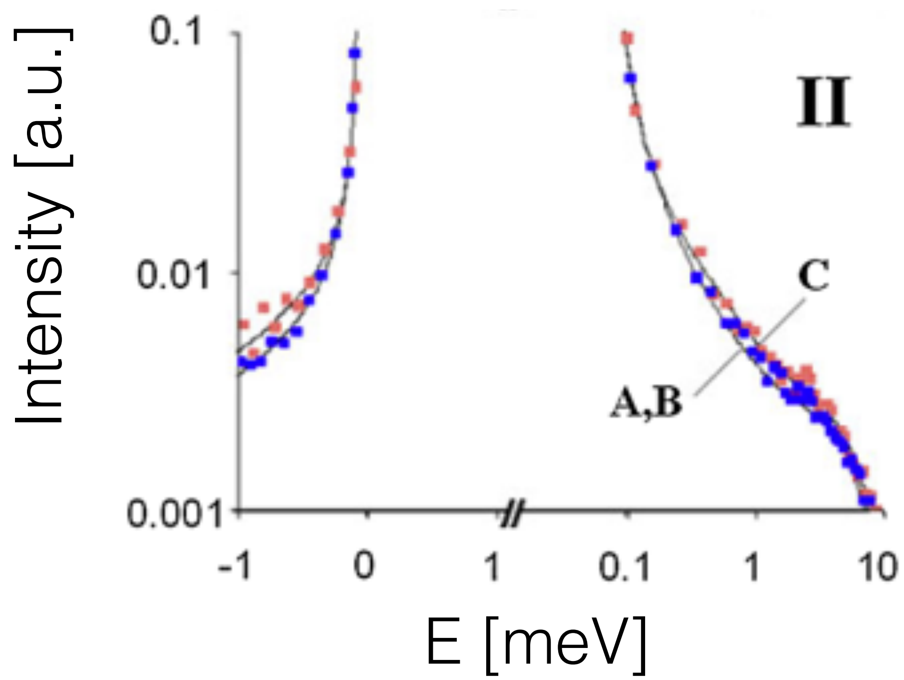
Figure 1. Photocycle of BR at room temperature. The ground state and the intermediates (J, K, L, M, N, O) are characterized by their absorption maxima (subscripts indicate the corresponding wavelengths in [nm]) and decay times. The inset shows the structures of a BR monomer in the ground state BR_{568} (purple) and in the M_{412}-intermediate (yellow), respectively, according to Sass *et al.* (4). Deprotonation and reprotonation of the Schiff's base are indicated by arrows.

Significance of protein structural flexibility, which is correlated with the large-scale structural changes in the protein structure occurring during the M-intermediate.

Time dependent laser pump probe studies of proteins.

A temporary alteration in both diffusive and vibrational protein dynamics during the proton pumping process in the membrane protein BR has been observed for the first time.



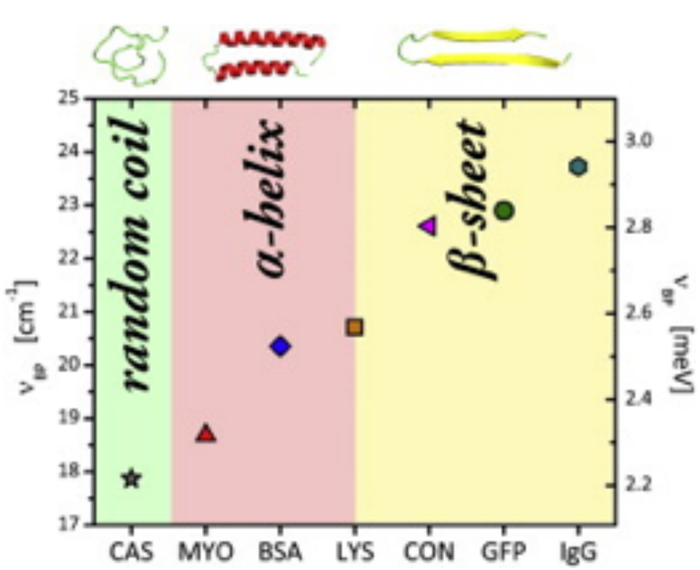


Technical difficulties:
Temporal synchronization of the QENS measurement with laser excitation
Exciting complete sample (20 % in this experiment)
Overcome signal to noise (56 pulses, several samples & full Q integration)

C-Spec

Dynamics of Soft Materials and Molecular Biophysics
Collective dynamics is a major property of soft matter

A. Sokolov ORNL
University of Tennessee,
USA Governor's Chair



Biophysical Journal
Cell PRESS
Volume 105, Issue 9, 5 November 2013, Pages 2182–2187

Article

Coherent Neutron Scattering and Collective Dynamics in the Protein, GFP

Jonathan D. Nickels[†, §], Stefania Perticaroli[‡, §], Hugh O'Neill[¶], Qiu Zhang[¶], Georg Ehlers[‖], Alexei P. Sokolov[†, §]

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http://dx.doi.org/10.1016/j.bpj.2013.09.029

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Biophysical Journal
Cell PRESS
Volume 106, Issue 12, 17 June 2014, Pages 2667–2674

Article

Rigidity, Secondary Structure, and the Universality of the Boson Peak in Proteins

Stefania Perticaroli[†, ‡, §], Jonathan D. Nickels[†, §], Georg Ehlers[¶], Alexei P. Sokolov[†, ‡, §]

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http://dx.doi.org/10.1016/j.bpj.2014.05.009

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University of Tennessee,
USA Governor's Chair

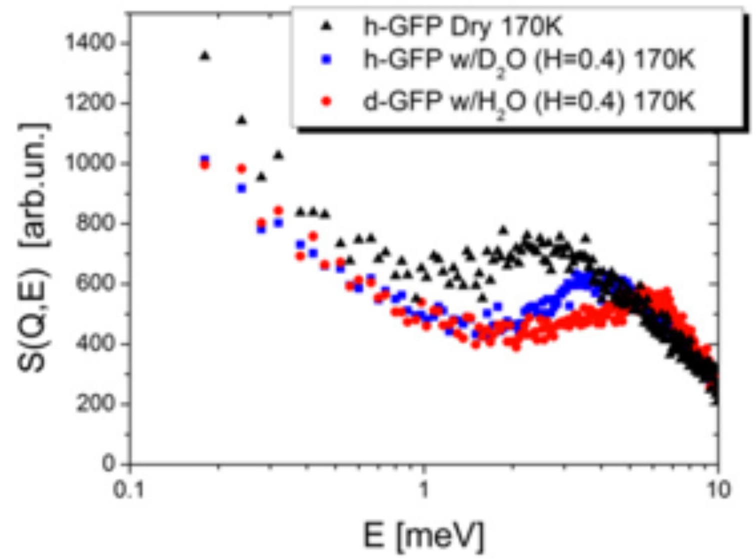


FIGURE 6 Dynamic structure factor from inelastic neutron scattering of d-GFP/H_2O (*red circles*), h-GFP/D_2O (*blue squares*), and dry h-GFP (*black triangles*) samples at $T = 170$ K. The spectra are summed over all measured Q (0.5–5 $Å^{-1}$). Dry h-GFP shows the highest QENS spectrum at $E < 1$ meV.

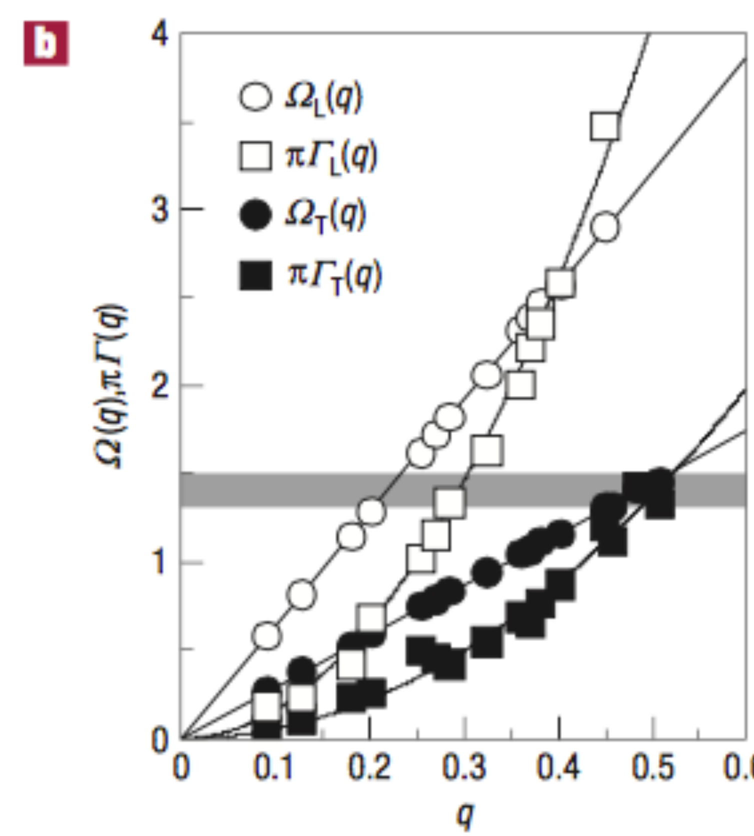
Biophysical Journal 103(7) 1566–1575

Unxepected low coherence of atomic motions in Green Fluorescent Protein. Low amount of in-phase collective motion of the secondary structural units contributing to the boson peak vibrations and fast conformal fluctuations on the picosecond timescale.

ARTICLES

Universal link between the boson peak and transverse phonons in glass

HIROSHI SHINTANI AND HAJIME TANAKA*
Institute of Industrial Science, University of Tokyo, 4-6-1 Komaba, Meguro-ku, Tokyo 153-8505, Japan
*e-mail: tanaka@iis.u-tokyo.ac.jp



Requirements:

Protein dynamics using various levels of deuteration. Currently requires 100 mg = too big & too costly. Reducing sample to 1 - 10 mg opens up totally new avenues of protein dynamics. GOOD SIGNAL/NOISE

Need high signal to kinetics of processes such as annealing/aging (56 pulses on IN5) GOOD SIGNAL/NOISE, LARGE DETECTOR AREA, OPTIMISED SAMPLE ENVIRONMENT

Wish to perform measurements at even higher energy resolution using higher wavelengths. HIGH FLUX

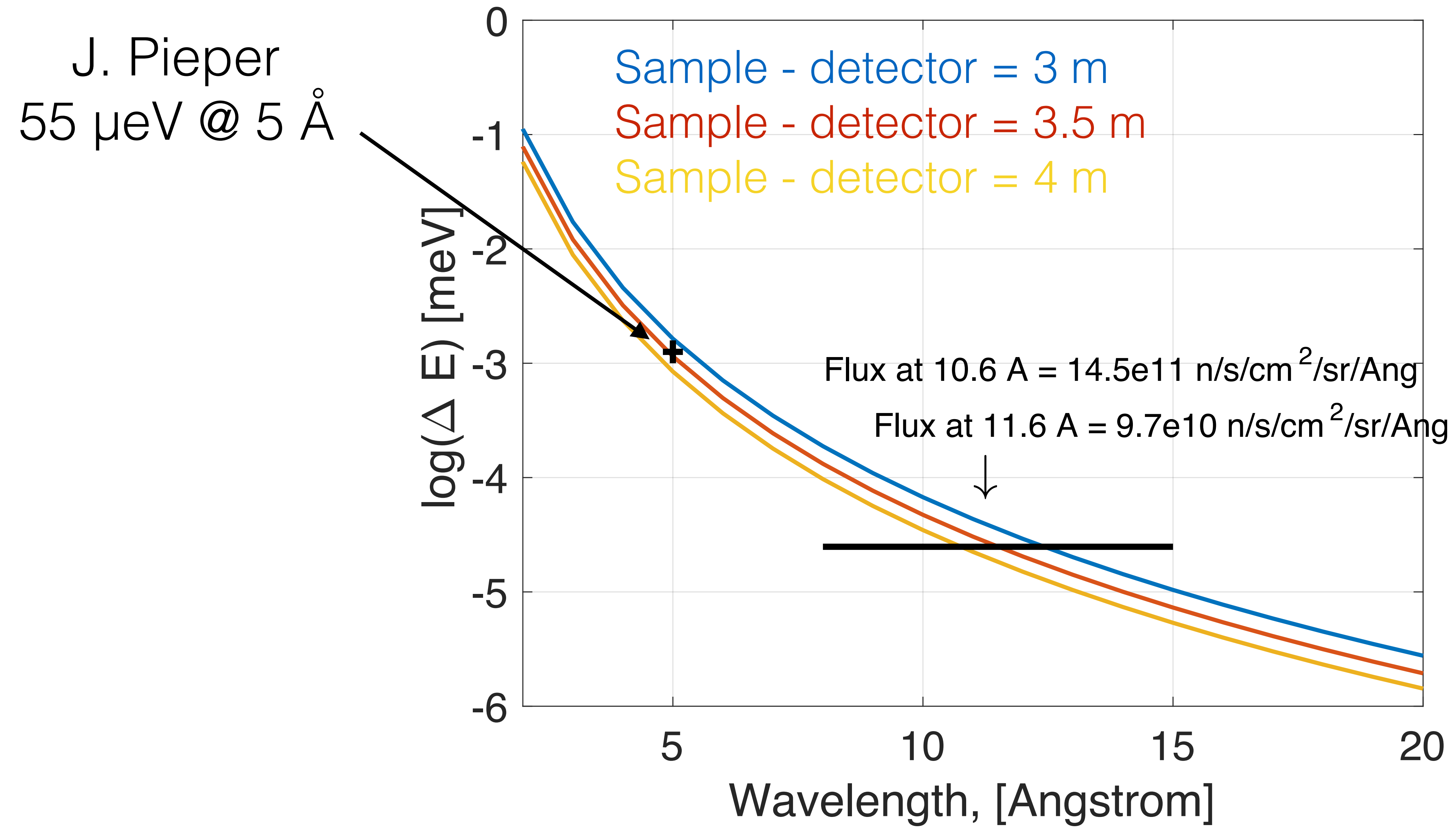
Q dependence - important for coherent scattering. LARGE DETECTOR AREA

Bottleneck is time to change and stabilise the sample temperature. Wasting half beam time on that. SAMPLE CHANGER

C-Spec

Requirements on energy resolution: Optimised primary spectrometer w.r.t. ESS pulse length, balanced to secondary spectrometer gives LSD = 4 m

Optimise energy resolution to cost, LSD = 3.5 m



(a) Sample to detector 3.5 m, similar to todays energy resolutions

(b) At high λ, reducing the distance by 0.5 m = loss of 1 order of magn. in flux.

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Frustrated magnetism

LETTERS
PUBLISHED ONLINE: 4 APRIL 2016 | DOI: 10.1038/NPHYS3710
nature physics

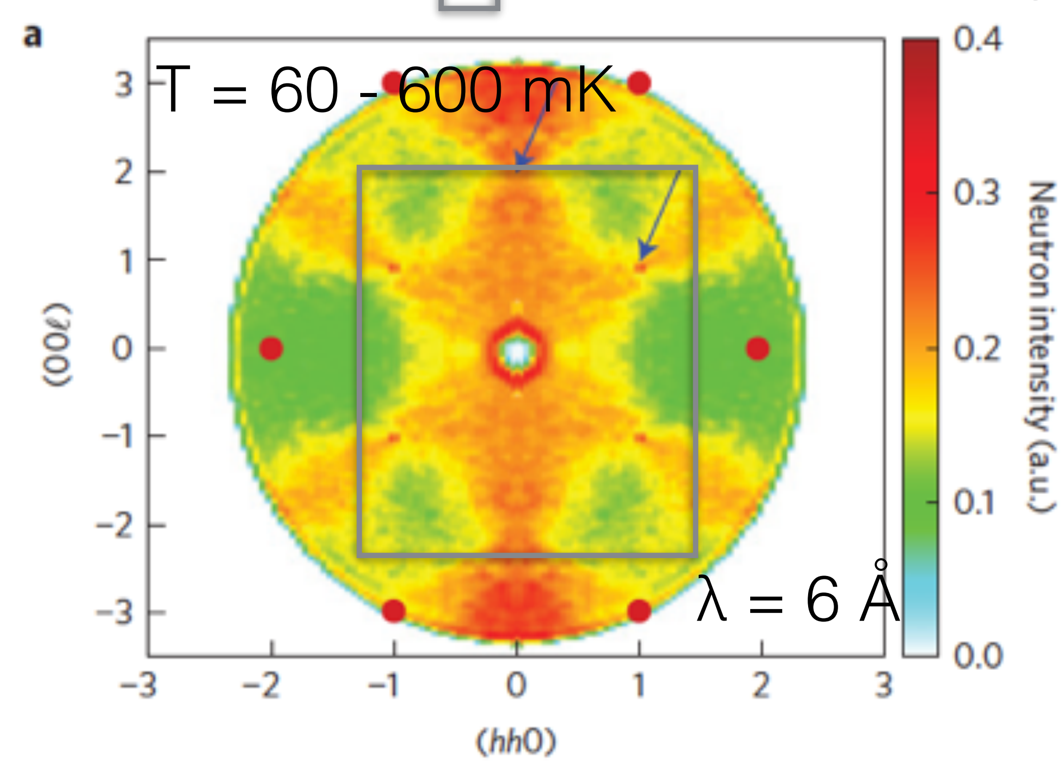
Observation of magnetic fragmentation in spin ice

S. Petit[1*], E. Lhotel[2*], B. Canals[2], M. Ciomaga Hatnean[3], J. Ollivier[4], H. Mutka[4], E. Ressouche[5], A. R. Wildes[4], M. R. Lees[3] and G. Balakrishnan[3]

Superposition of magnetic Bragg peaks (ordered phase) and a pinch point pattern (Coulombic monopole phase).

Relevance of the fragmentation concept to describe the physics of systems that are simultaneously ordered and fluctuating.

$Nd_2Zr_2O_7$ □ = 70° detector coverage



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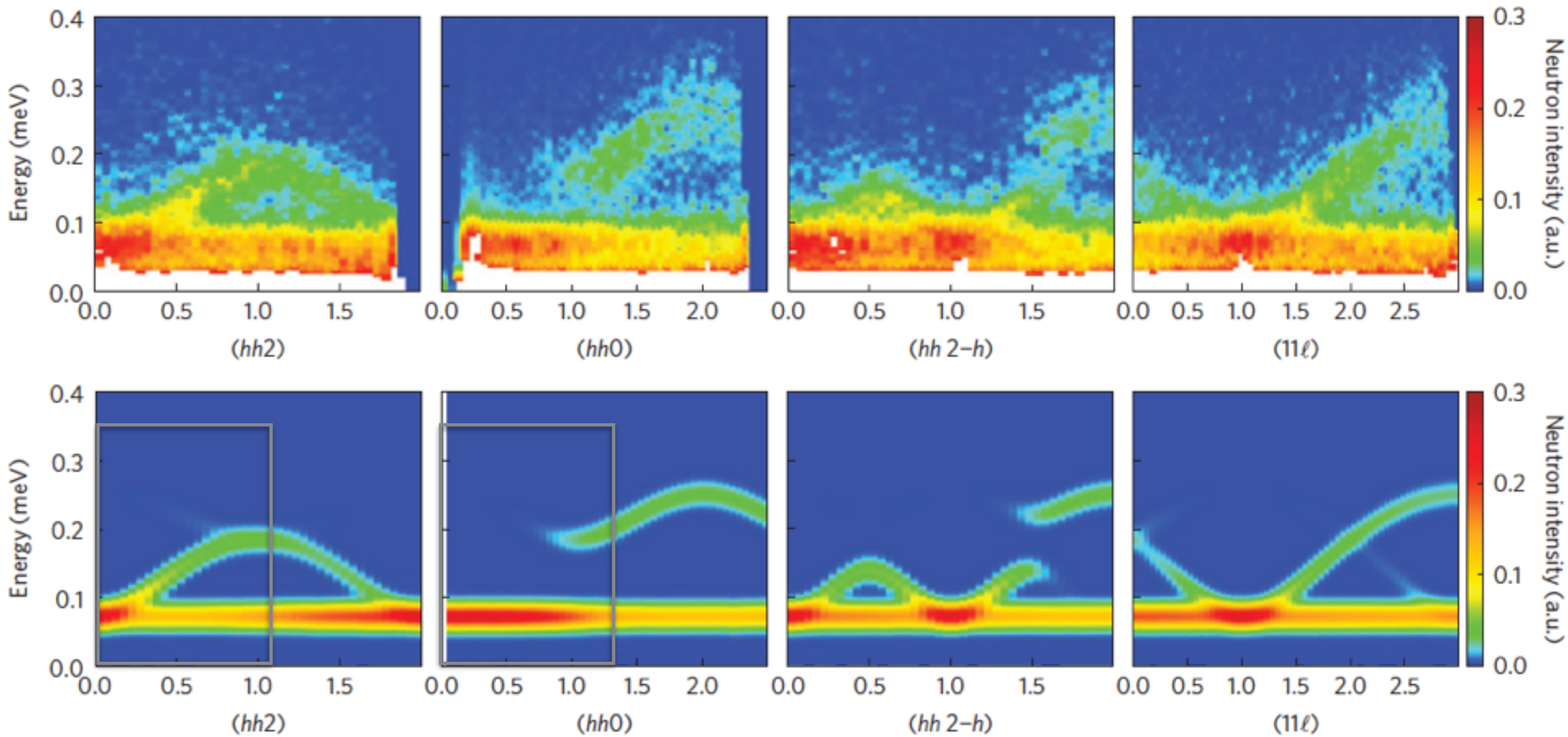
S(**Q**, ω)

□ = 70º detector coverage

sample rotated by steps of 1 degree (1 - 130º) - sample rotation stage

Modes persist up to 600 mK - dedicated low temperature eqp.



Organic molecules

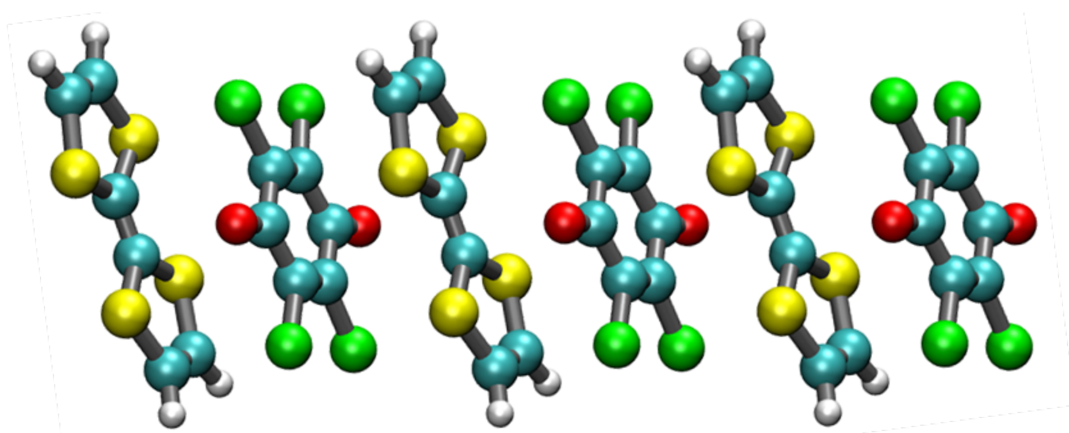
Hydrogen-Bonded Charge Transfer Crystals: Room Temperature Ferroelectrics

M. Masino, G. d'Avino, Parma University, Mons University

PRL 99, 156407 (2007) PHYSICAL REVIEW LETTERS week ending 12 OCTOBER 2007

Anomalous Dispersion of Optical Phonons at the Neutral-Ionic Transition: Evidence from Diffuse X-Ray Scattering

Rich physics: complex phase diagrams, competing phases, quantum phase transitions.



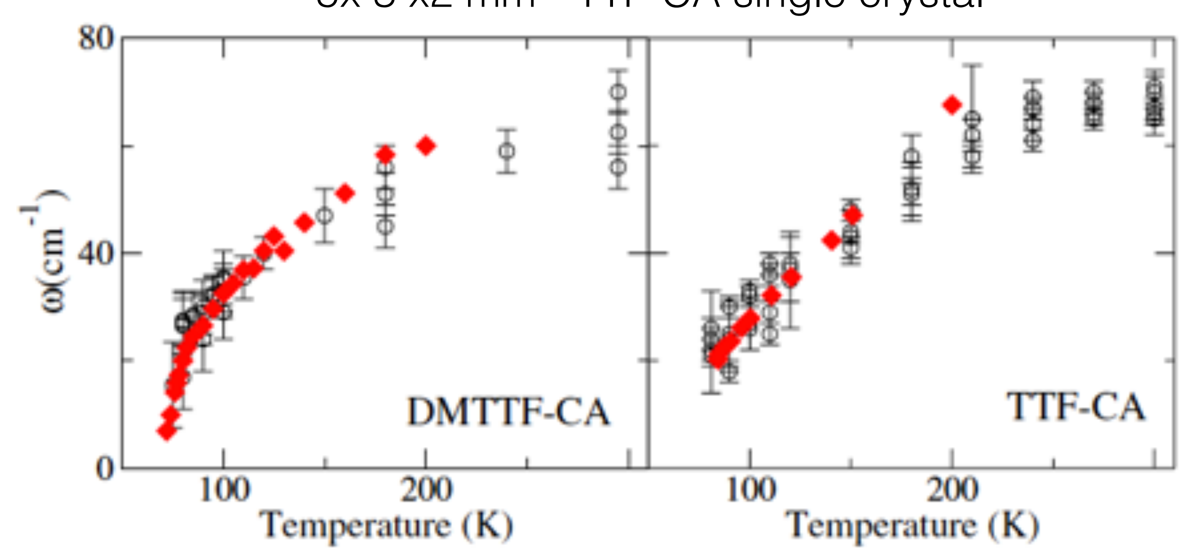
D A D A D A

C , Cl, H, O, S

Solitons and domain boundaries are intriguing low-energy excitations in 1D systems such as organic charge-transfer (CT) salts.

Photo-induced transformations, relaxation of optically excited states results in structural and electronic orders. Electronic-structural coupling leads to high conductivity ⇔ low conductivity states

5x 3 x2 mm³ TTF-CA single crystal



Requirements:

New physics manifests itself as broad features superimposed on sharp features.
GOOD DETECTOR COVERAGE

Broad features can be difficult to separate from background features.
EXCELLENT SIGNAL TO NOISE

Samples are difficult to synthesise - small samples.
REQUIRES FOCUSSING NOSE

Interesting physics is at low temperatures, DILUTION ESSENTIAL

Make it possible to probe out of equilibrium phenomena
ACCESSIBLE SAMPLE ENVIRONMENT, EXCELLENT SIGNAL/NOISE

Organic compounds, high H content. POLARISATION ANALYSIS
MUST BE AVAILABLE WITHIN A FEW YEARS

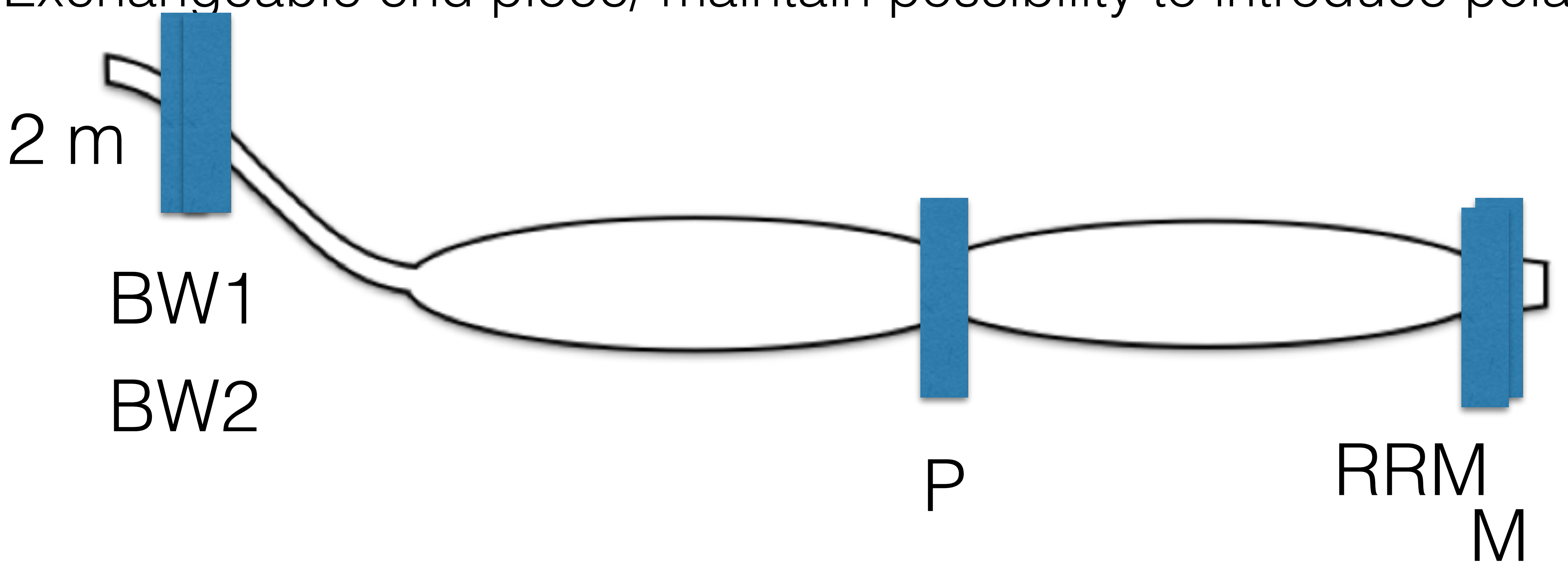
Overview:

Science case & requirements
Beam extraction & Guide
Choppers
Detector tank
Sample environment
Beam stop
Shielding
Costing
Budget & Overview

C-Spec

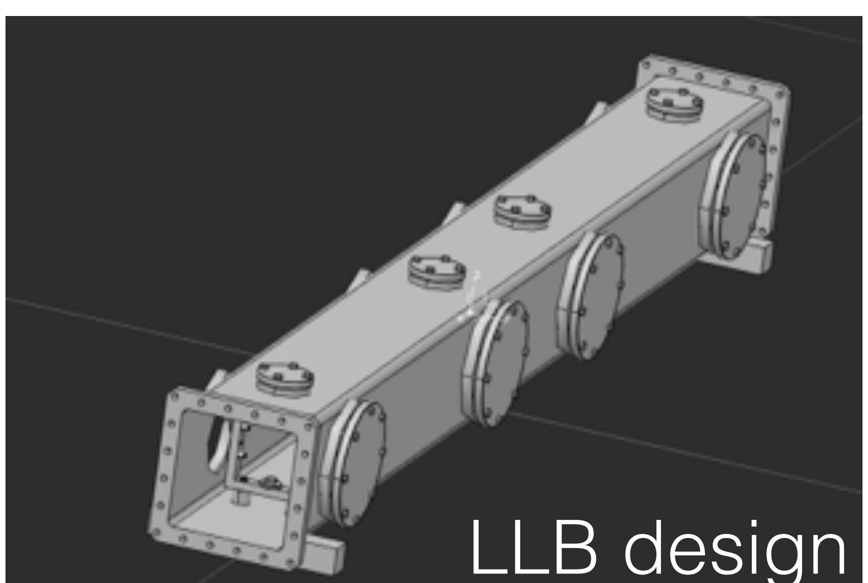
Guide Requirements:

- Focus on cold moderator (2 - 20 Å).
- Optimise for signal to noise.
- Divergence +/- 1^{o} at 3 Å.
- Width ~ up to 10 cm at P chopper.
- Width ~ 14 mm at M chopper ΔE/E=1 - 4%
- Focus to (a) 4 x 2 cm^2, (b) several mm^2
- M values mostly < 3
- Exchangeable end piece/ maintain possibility to introduce polarising guide



C-Spec

Cost (no VAT): 3150 k€
= Guide (2450 k€)
= external Vacuum housing (600 k€)
= installation (100 k€)



quote: Swiss neutronics

Overview:

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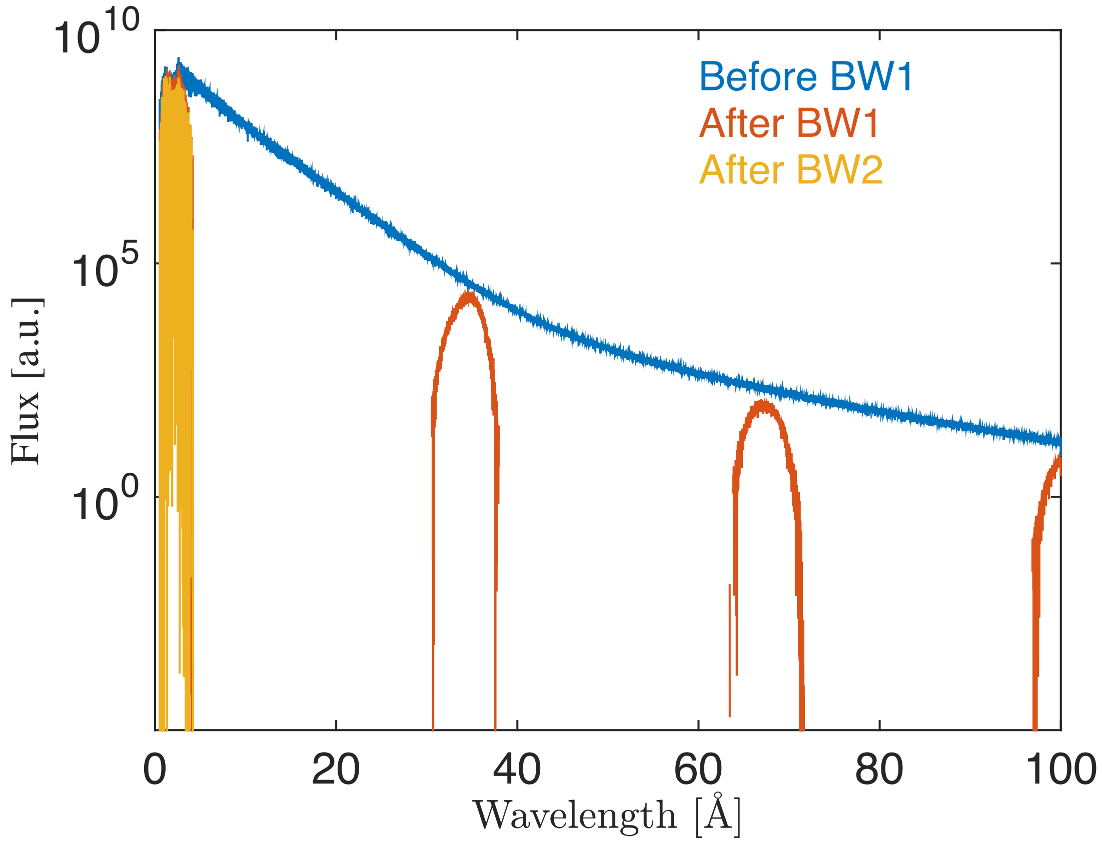
Choppers

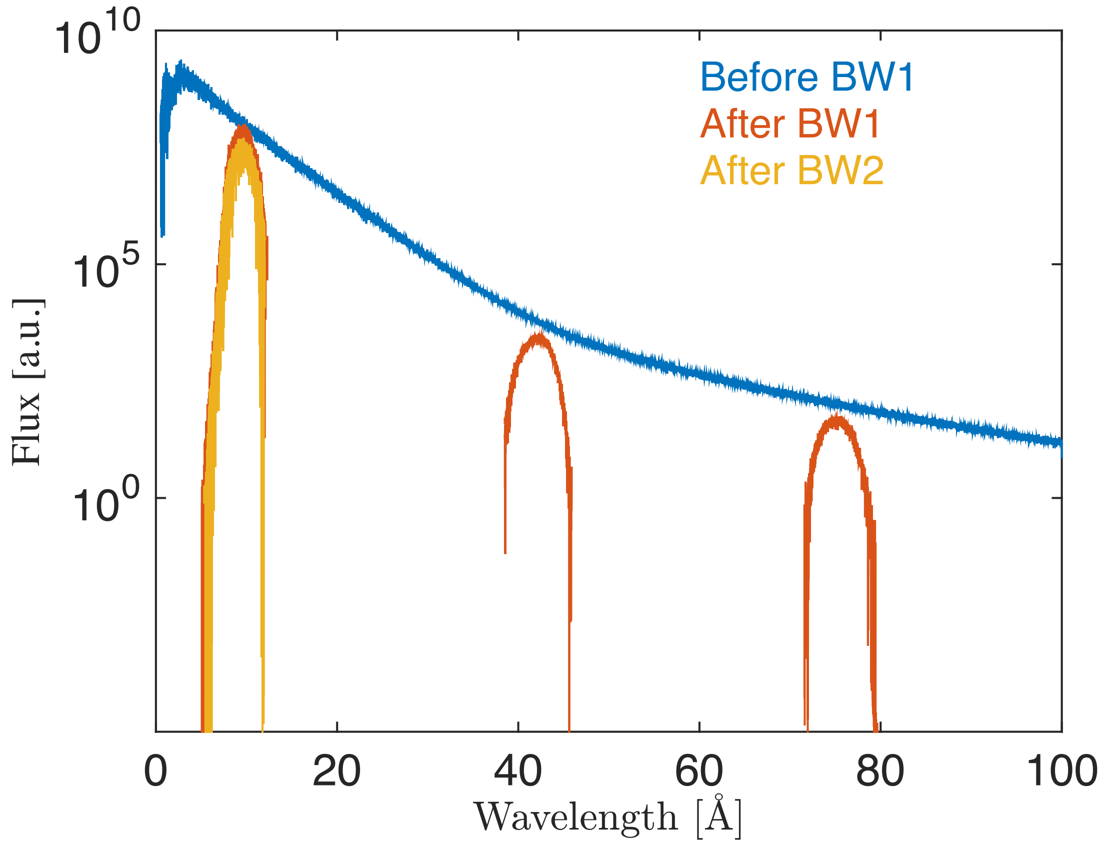
Chopper Name	Position (m)	Single Blade (SB) or	Diameter (mm)	Number of openings & slit	Max Frequency (Hz)	Absorber	Bearing
BandWidth 1	8.5	SB	700	1 & 16°	14	Metallic (B coated)	Hybrid ball bearings
BandWidth 2	10	SB	700	1 & 29°	14	Metallic (B coated)	Hybrid ball bearings
Al2O3 Block/ T0 chopper	**50**						
Pulse Shaping	~Mono*2/3	CR	600	3 & 23°	350	Carbon fibre (B coated)	Magnetic
Mono_RRM	Mono-0.05	SB	600	1 & 2.6 °	350	Carbon fibre (B coated)	Magnetic
Monochromating 2 x(double Slit)	~Mono	CR	600	1 & 2.6°	350	Carbon fibre (B coated)	Magnetic

Bandwidth choppers at 8.5 & 10 m

$\lambda = 2$



$\lambda = 8$ Å

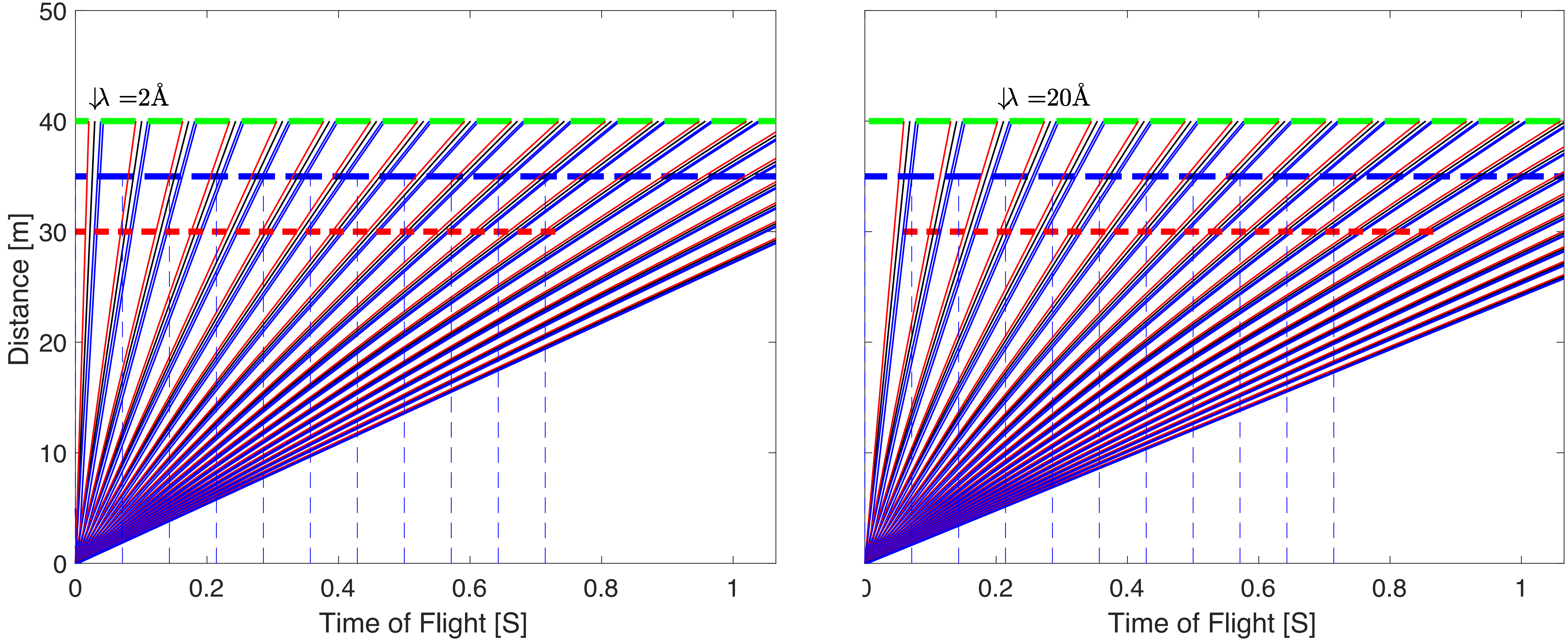


Bandwidth choppers: prompt pulse reduction.
Need more information on prompt pulse

McStas 2.2a

C-Spec

STAP request to play BW choppers outside bunker



Possible

Requires 3 BW choppers.

Analytically clean up to 60 Å.

Preferred option is BW within the bunker

Cost: 1320 k€ (Airbus)

BW choppers with metal disc and B4C coating, 600 mm diameter, 14 Hz, Hybrid Ball bearings: 120 k€/each
BW choppers with metal disc and B4C coating, 700 mm diameter, 14 Hz, Hybrid Ball bearings: 125 k€/each

Triple chopper with CFRP disc, B10 coating, 600 mm diameter, 350 Hz, magnetic bearings: 650 k€

Double chopper with CFRP disc, B10 coating, 600 mm diameter, 350 Hz magnetic bearing; 420 k€

The prices above are calculated as three chopper systems (BW, PS, Mono). Each system will have one control and one monitoring system.
The prices are also including the onsite commissioning at ESS in Lund.
The prices are based on the efforts for paperwork and documentation of already delivered systems in the past (TOFTOF)

From chopper group:

Double disk chopper (700 mm, speeds above 196 Hz): 280
Chopper integration module : 33
Drives and power 5
Installation 17
Integration 15
Commisioning 10
Power system 30
Vacuum 5
Chopper cooling 10
Master rack x2 15
Slave rack 7

We have 420 k€ for a Double Disk chopper

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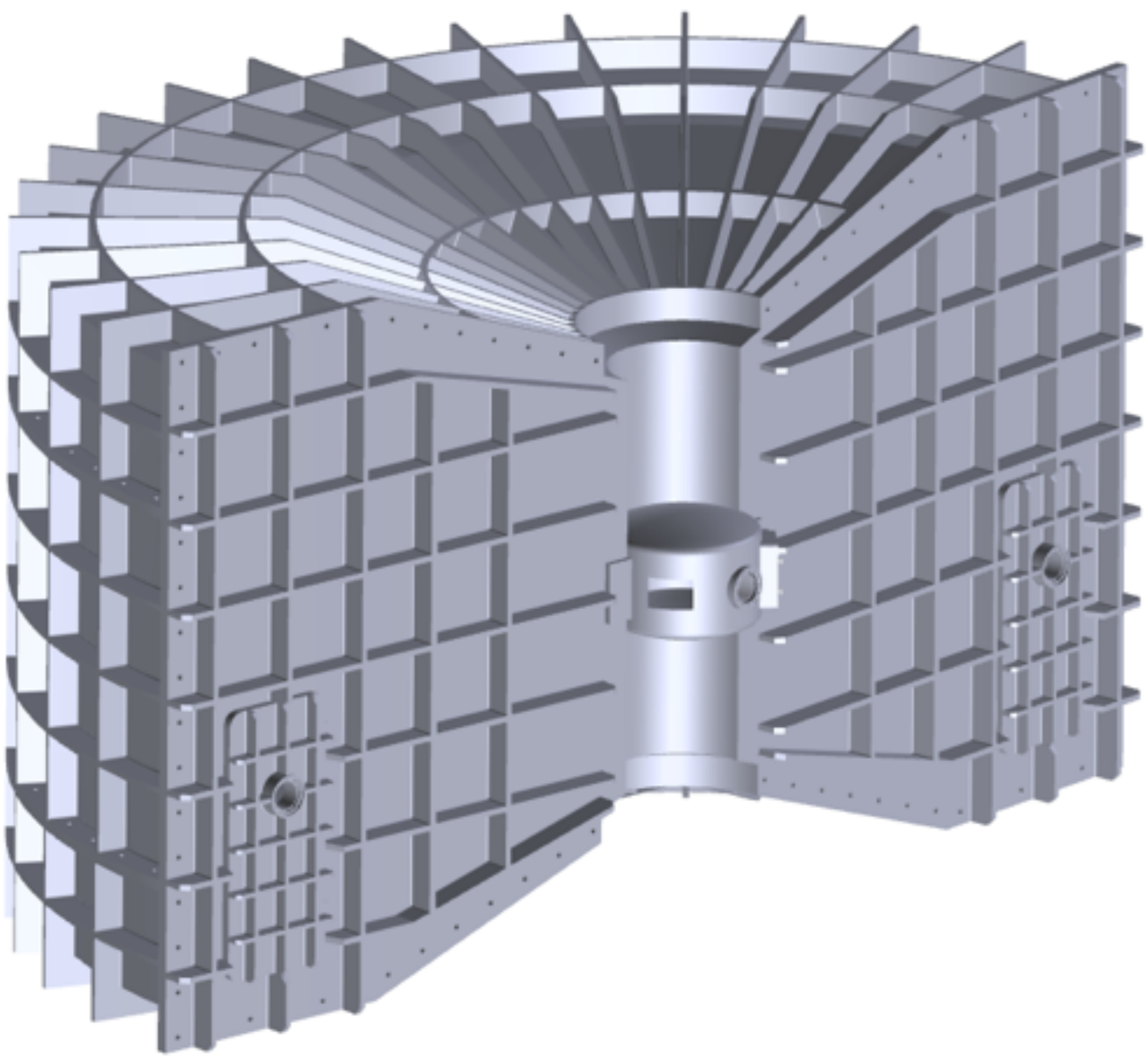
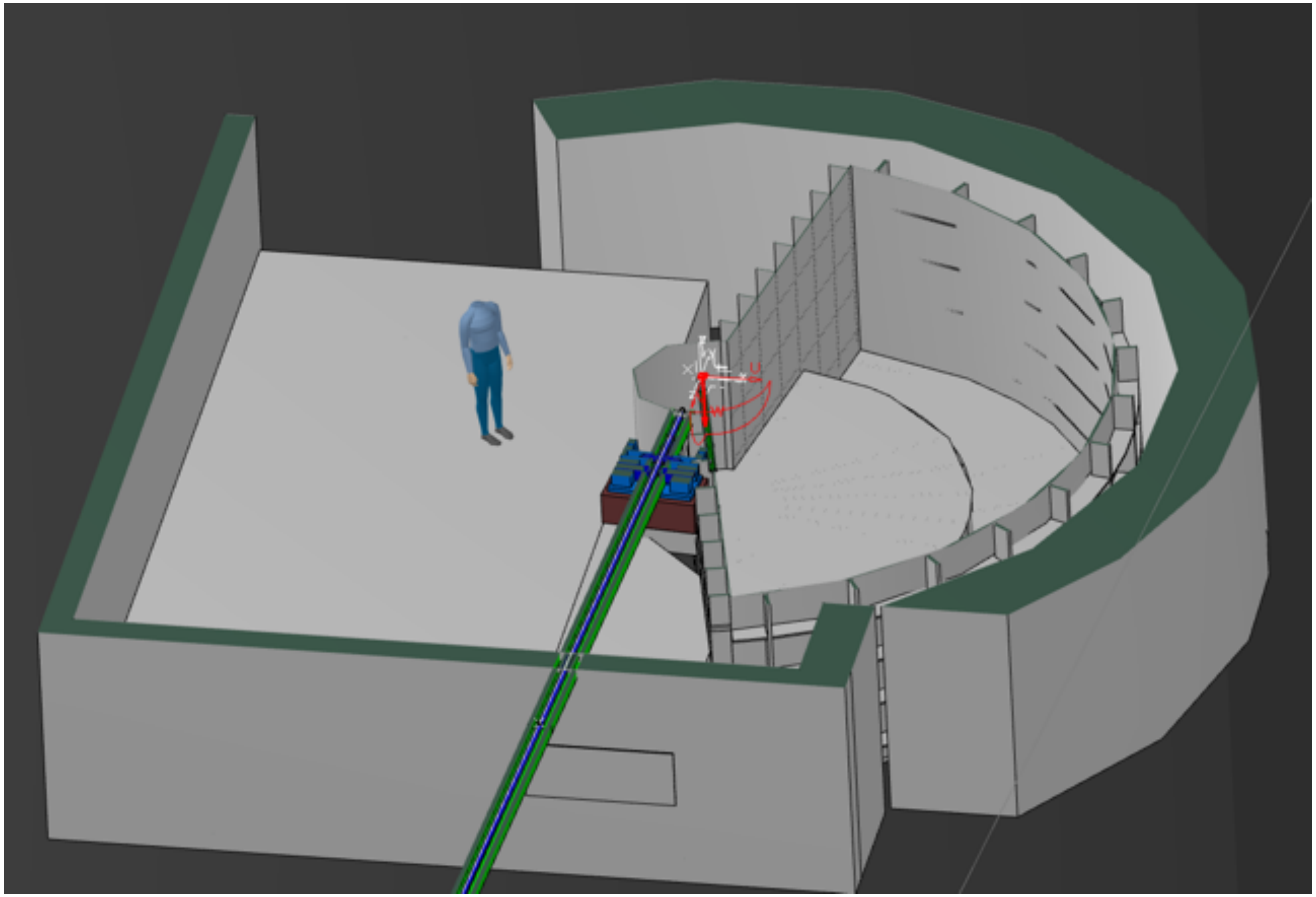
Detector tank



Tank:
Sample - Detector = 3.5 m, 4 m height
angular range 5 - 140° (image pre-stap)
Non-magnetic
Pressure = 10^{-6}
Implementation of detector array

Sample environment:
1 m radius
Pressure = 10^{-6} to inert atmosphere
accessible from top/side
Optimised for in-situ studies

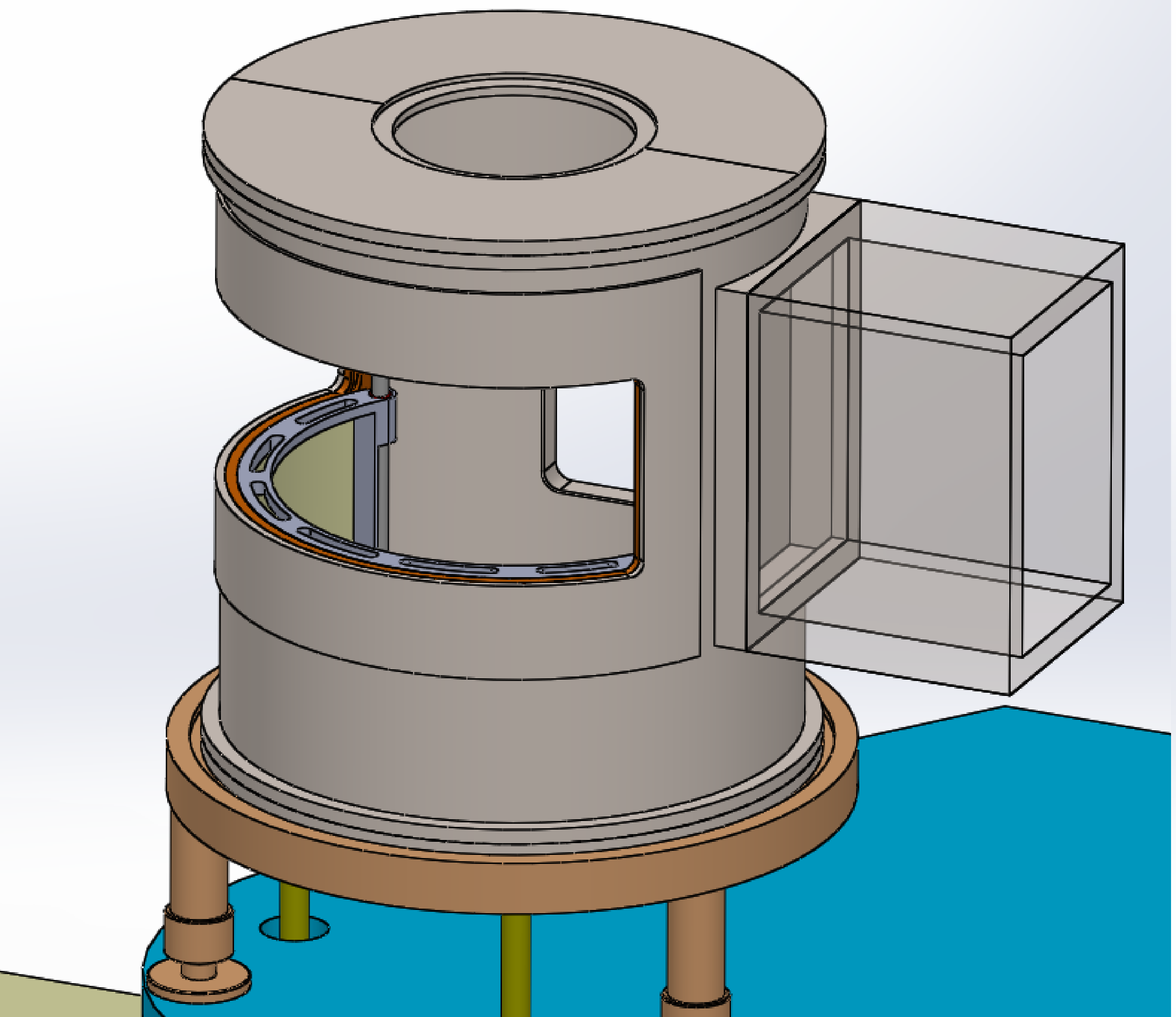
Detector tank (half height shown)

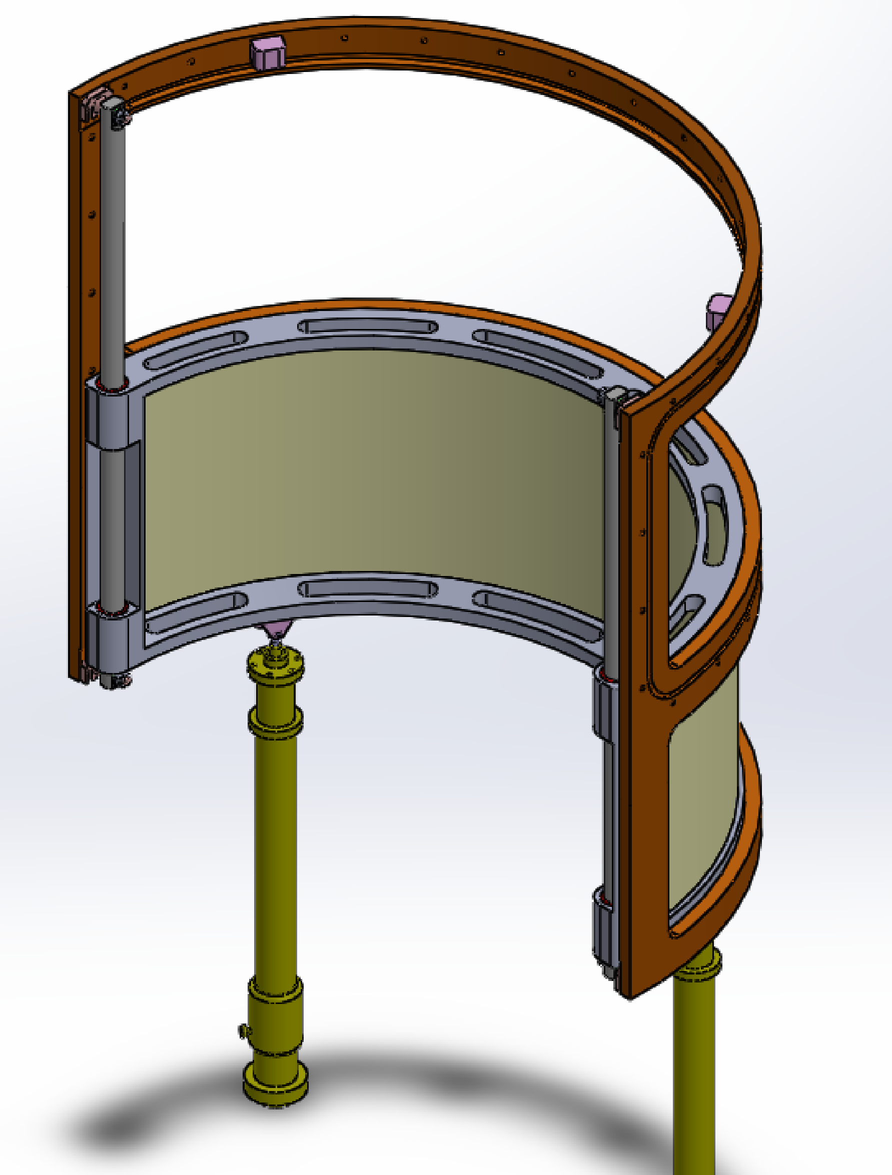


Last window: Monochromatic chopper
Guide exit within sample environment area
Details of Collimator under consideration

Sample environment space within detector tank:

Requirements:Access from side
Cryogenic vacuum & ambient
If B^{10} detectors - static pressure in main vacuum tank
In-house experience (TUM & LLB)





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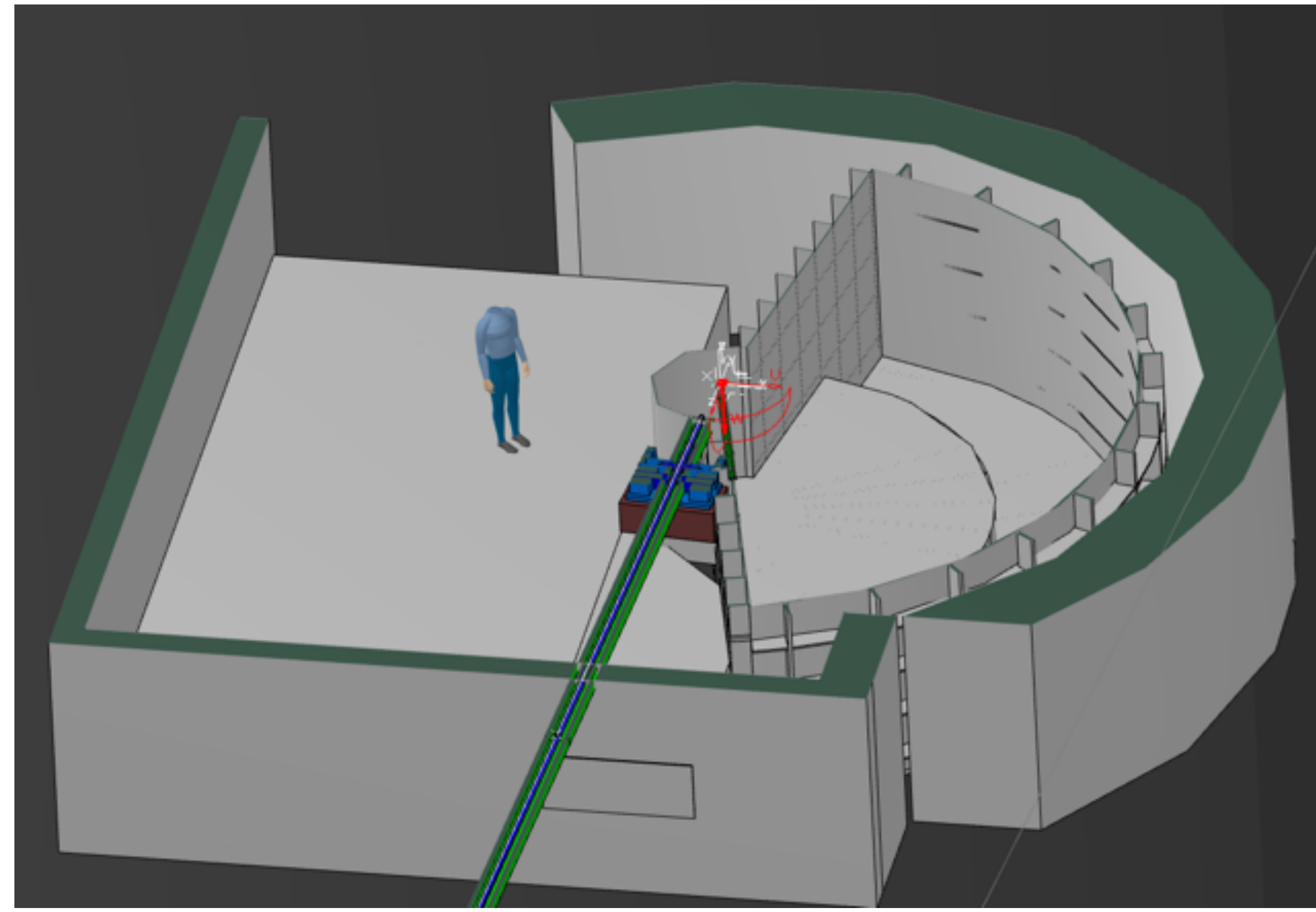
Detector tank



Cost: 1626 k€

Includes radial collimator.

Cadmium sheets.

Manpower.

design department of LLB (collaboration with SDMS Fa#& PA20 @ LLB)

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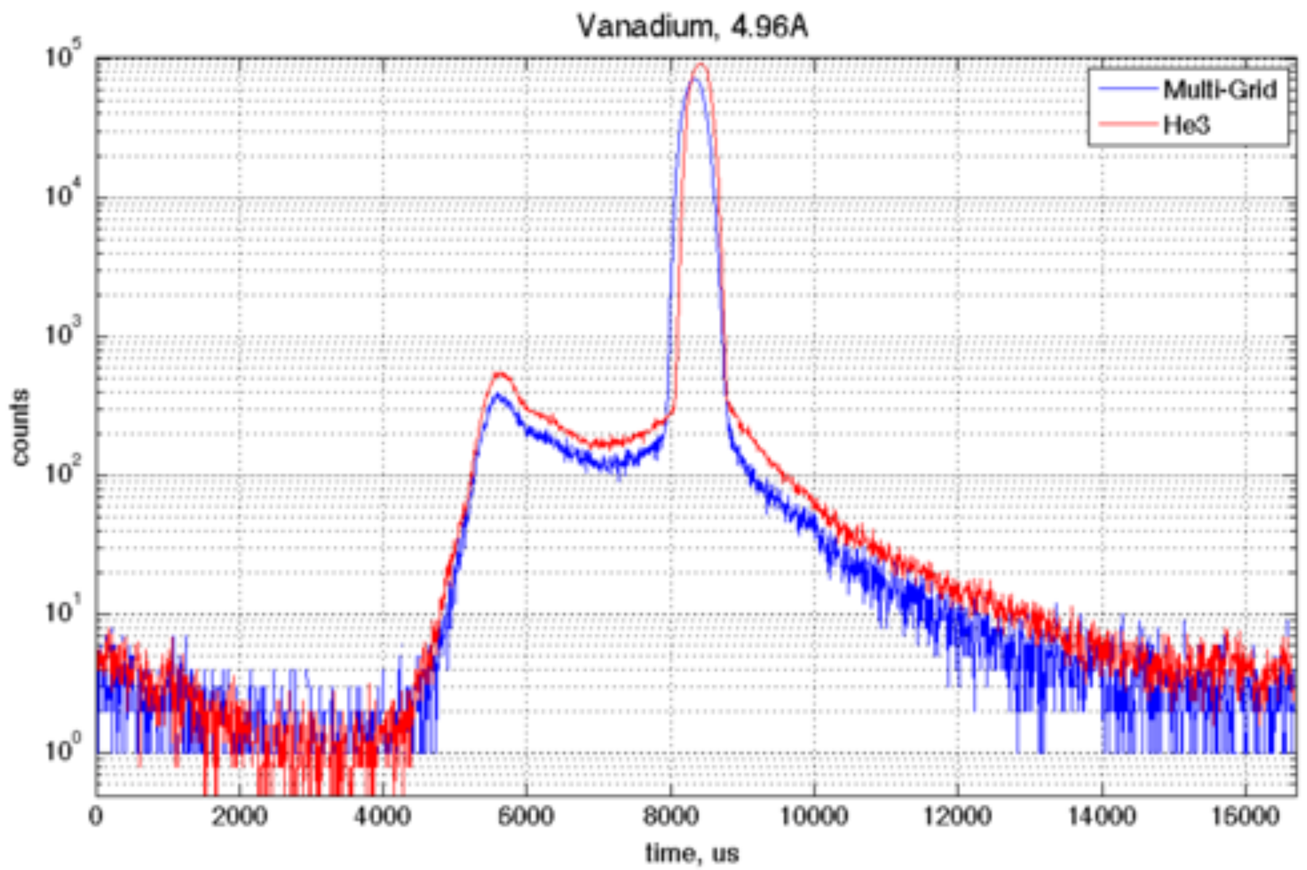
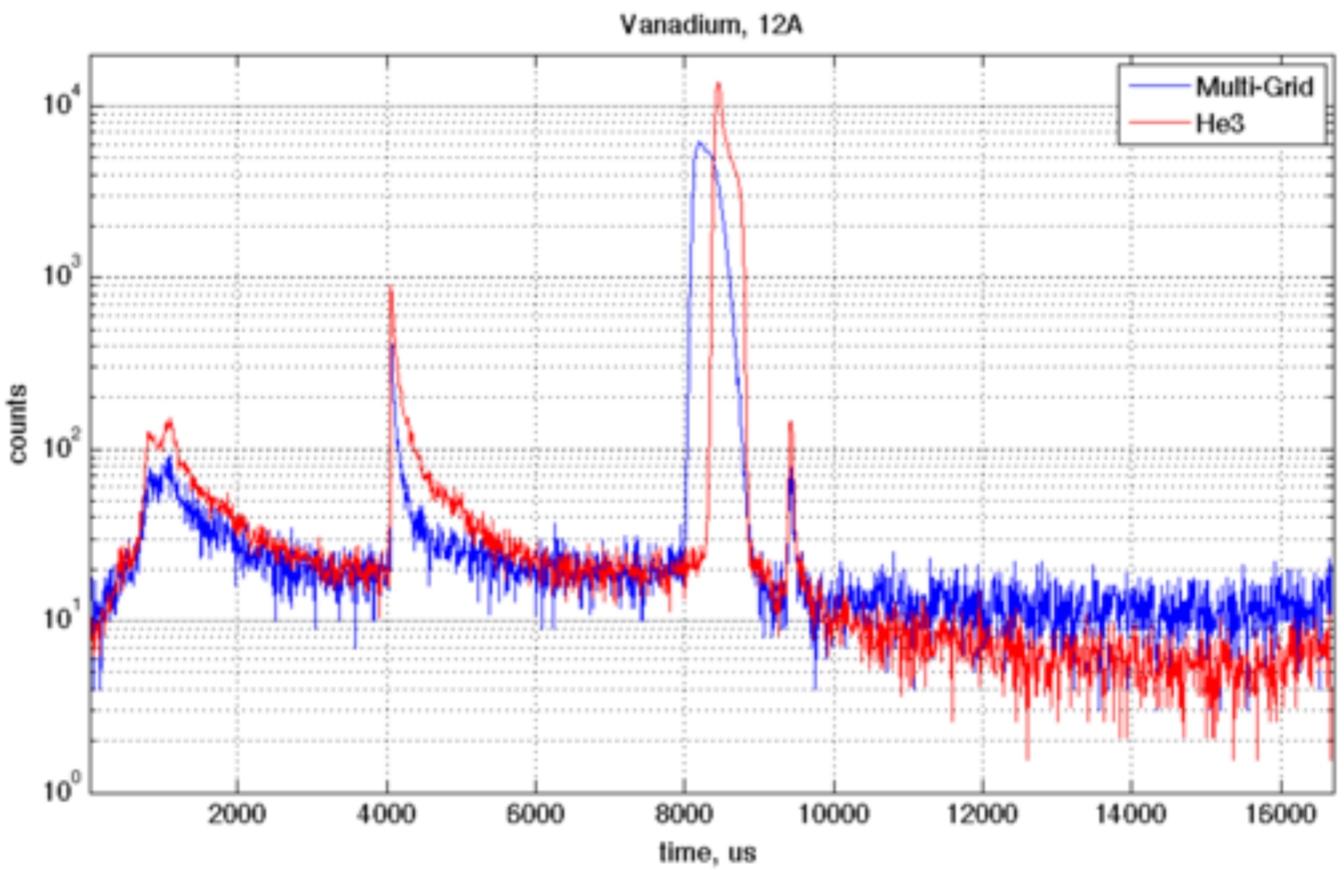
Detector technology: B10.





B10 multigrid at CNCS (SNS) (comparison with 6 bar He3)
Great success
More tests needed.

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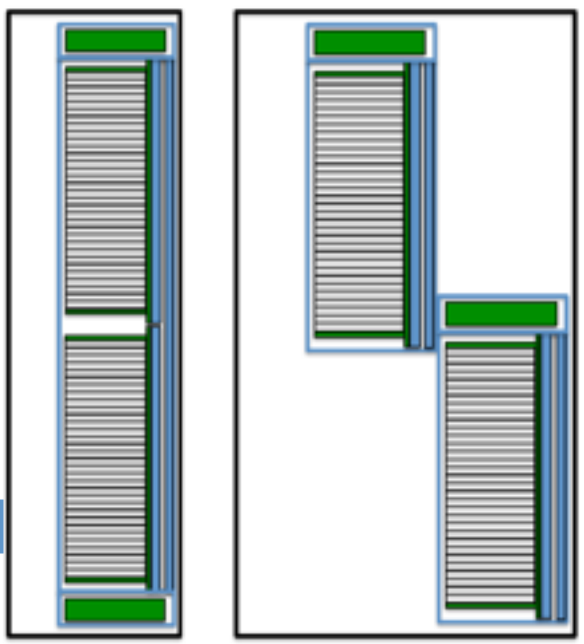
Detector technology: B10.

STAP: Continuous coverage with NO gaps
STAP: Try to cover horizontally first,
then focus on vertical coverage



CSPEC configuration	33m2 16-layer	33m2 16-layer 2-bank
Coating are, m2	1056	1056
Coating margin, m2	106	106
Coating tot, kEur	1596	1596
Grids # channels	12800	12800
Wires # channels	**5150**	**10240**
FEE tot, kEur	**1792**	**2304**
BEE tot, kEur	200	200
HV+LV tot, kEur	200	200
Grids #	12800	12800
Work+material tot, kEur	**474**	**592**
Assembly+wiring, work	1 MW/col	1 MW/com
Wires #/col	64	64
Assembly+wiring, kEur	**154**	**308**
Column mechanics, kEur	**133**	**266**
Column shielding, kEur	**64**	**77**
Column support, kEur	**80**	**160**
Testing, kEur	**100**	**200**
Assembly, kEur	**100**	**200**
Services, kEur	50	50
Installation, cold commissioning	**186**	**372**
Tot, kEur	**5129**	**6525**

inconsistent with NO gaps.

1. Two 1/2-modules in single vessel

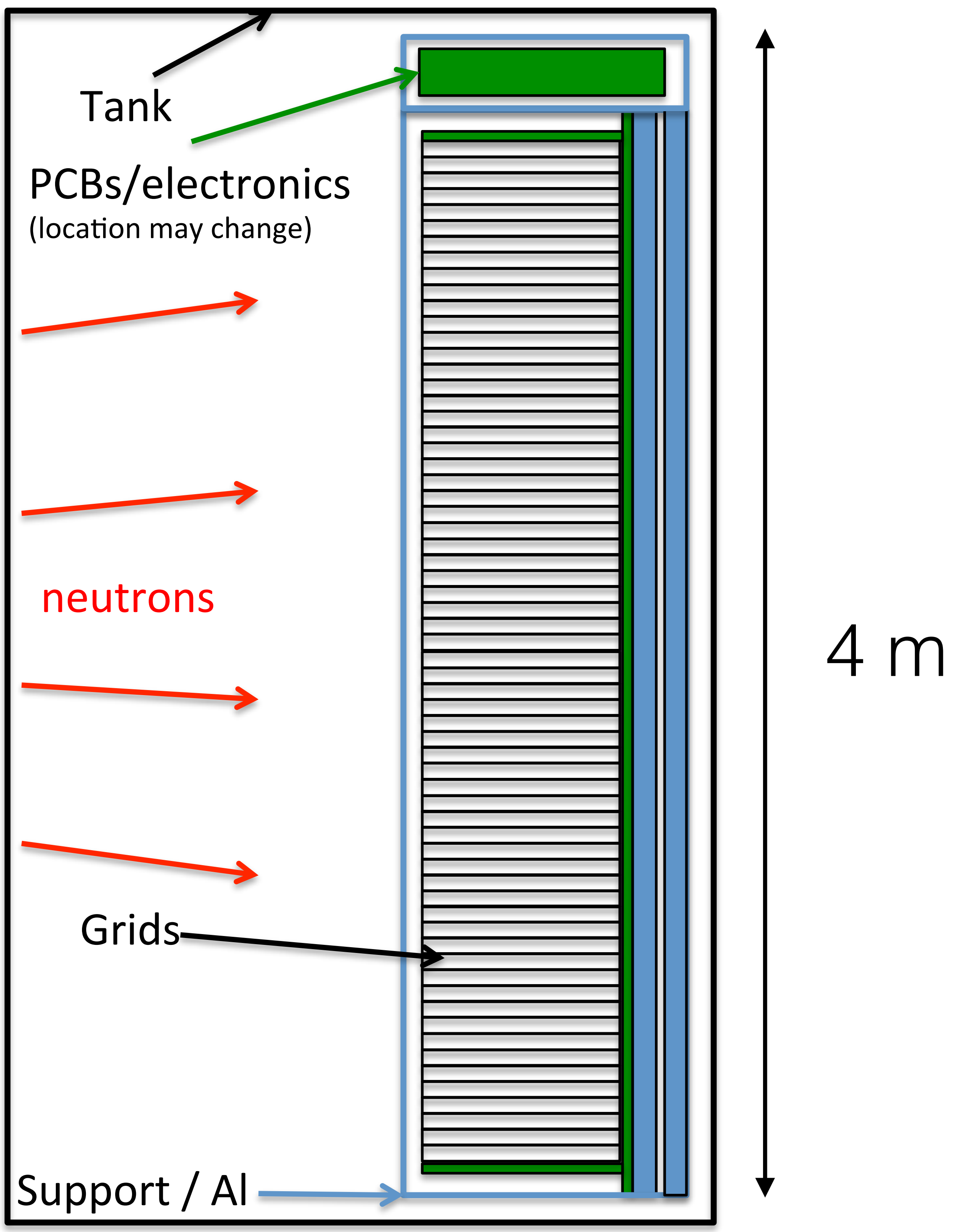
Disadvantages:

- Double the number of wires
  – approximately 50% more electronics channels.
- Both stacks need to be removed for service.
- Access to electronics both top and bottom of the detector.
- Full vessel and mechanics installed on day 1.
- Unused Ar volume.

Advantages (compared to option 2):

- Same sample distance.
- No vessel edge between stacks.

B10 Detectors, final solution



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C-Spec

EUROPEAN SPALLATION SOURCE

He3

GE Oil & Gas
Digital Solutions

BUDGETARY QUOTATION

To	Technische Universitat Munchen Boltzmannstr. 15 Garching B. Munchen, Bayern 85748 Germany Attn: Pascale Deen Email: pascale.deen@ess.se	**From**	8499 Darrow Road Twinsburg, Ohio 44087 U.S.A. T 330.963.2448 M 330.522.2035 E james.vogel@ge.com Reuter-Stokes, Inc.
Date	May 3, 2016	**Freight Terms**	FCA Twinsburg, OH
Quotation #	1505925 Rev 1	**Freight Charge**	Pre-Paid and Charged
Valid Through	August 31, 2016	**Payment Terms**	TBD

Detectors

Line	Item Number	Description	Qty.	Unit Price	Total Price
		With RS Supplied He3 Gas			
1	RS-P4-08158-204	Position Sensitive Neutron Detector	328	$12,000	$3,936,000
		1 inch Diameter x 157.9 inch Active Length			
		2 atm RS He3			
		Stainless Steel Body			
		Vacuum Coupling Connectors			

Will take decision on detector technology in February 2017

m^2 = 8167,2 k€

5 bar = optimal efficiency at low λ and short penetration length at high λ

Electronics

Line	Description			
	Deliverables			
1	80 preamplifiers (8 channel)			
2	20 signal processing modules including an RSPP and digitizer			
3	One set of prototype electronics consisting of two preamps, one digitizer and one RSPP			
4	Basic evaluation software			
5	One to two engineers after contract award to work with C-Spec engineers to finalize the electronics design			
6	One Engineer for up to one week to support initial prototype testing at TUM			
7	One Engineer for up to one week to supervise the electronics installation			
8	Reference and operating manuals			
			Total USD	**$1,200,000**

33 m^2 = 1,200 k€

Sample environment (full):

Scope 1, 2

Scope 3

Sample changer	150 k€
12 T magnet	0 k€
Cryofurnace	60 k€
Cryostat	60 k€
Dilution/He3 insert	175/110 k€
Sample rotation stage	5k€
Goniometer	5 k€
Huber goniometer (2 axes)	45 k€
Internal goniometer	20 k€
Optics for laser irradiation	75 k€
Gas handling panels	200 k€
Humidity chamber	40 k€
Total SE	910 k€

In-situ developments
Collaboration with J. Pieper
TOFTOF

Overview:

Science case & requirements
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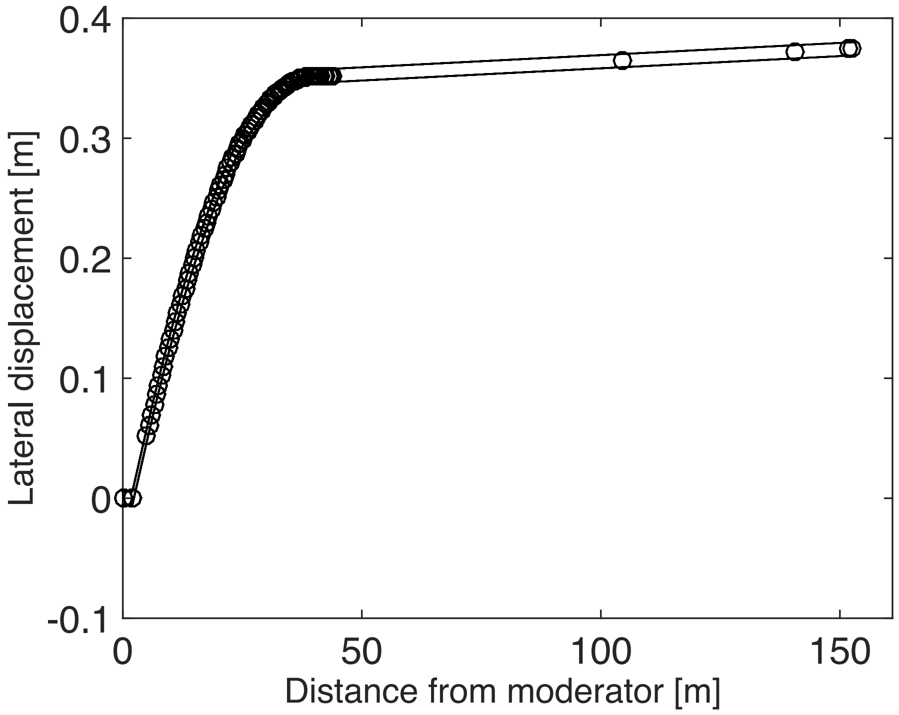
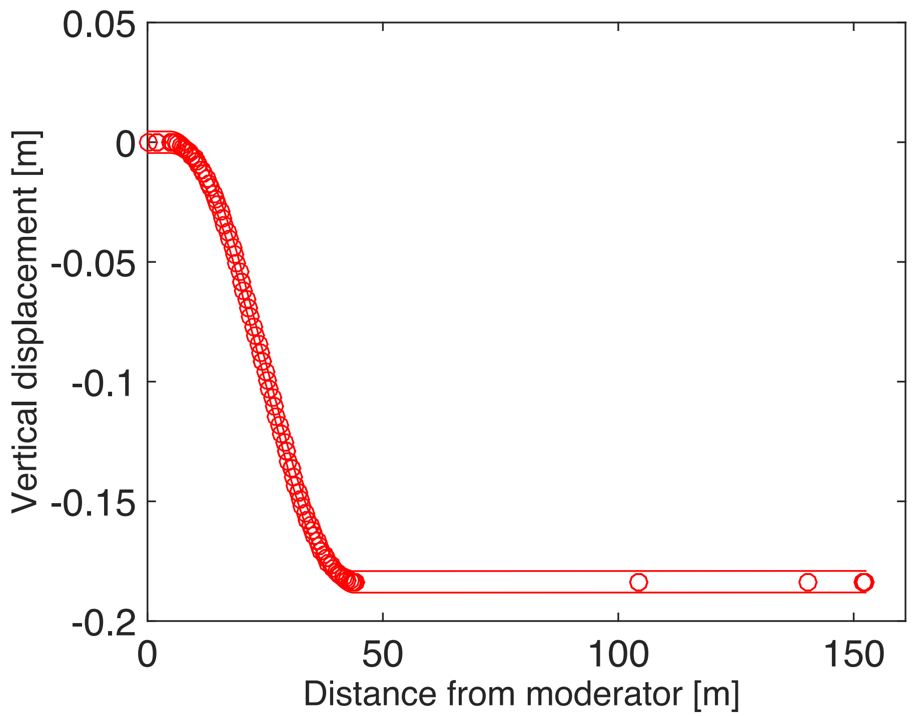
Sample environment
Beam stop
Shielding
Costing
Budget & Overview

Shielding



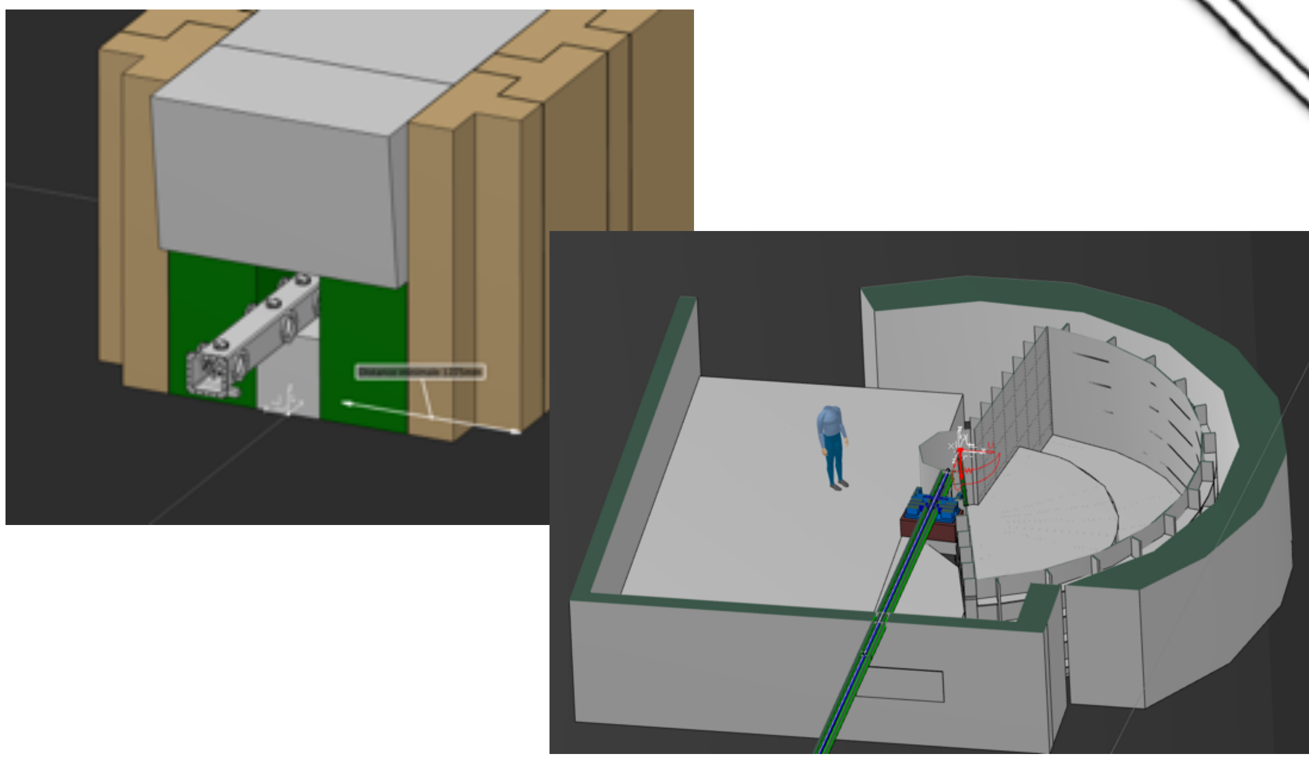


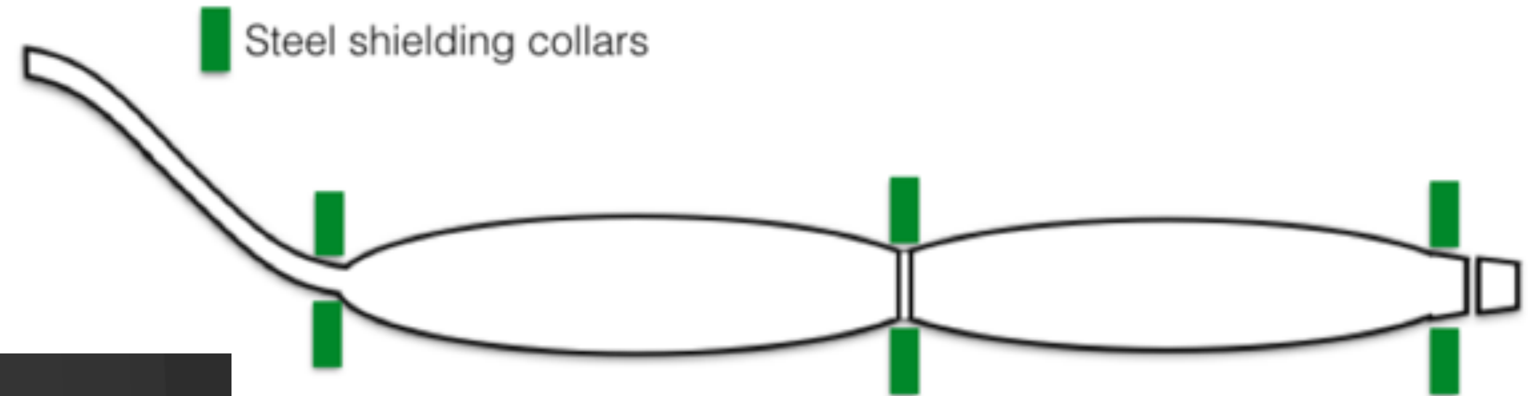
Optics group:

Beamline Shielding (m=2/3):
Out of line of sight: average Ni/Ti photon 4.4 MeV
40 cm steel equivalent, HD concrete: 80 cm

Cave Shielding: 30 cm steel equivalent calculated using 2 MeV photons, HD concrete: 60 cm

Shielding 1 129 k€





Guide & Detector 5 cm steel all round
Guide: 120 cm normal concrete
Guide 30 m - 40 m: additional 30 cm normal concrete
Detector tank: 85 cm normal concrete.
Including beamstop
Manpower = 5 months

1 k€/m^3 concrete (2300 kg/m^3) - 15.6 k€/m^3 steel (7800 kg/m^3)