A High Performance Hybrid Spectrometer for the Single Crystal Studies at the Pulsed SNS

BROOKHAVEN NATIONAL LABORATORY

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Outline

- HYSPEC project: history and general overview (motivation, scientific case, technical concept, etc).
- Instrument Development Team and current status of the project.
- Conceptual design and floor layout of the proposed instrument
- Overview of the results of MC simulations of instrument performance and comparison with the traditional TOF setup.
- HYSPEC summary, current issues and plans for future. HYSPEC Letter of Intent.

HYSPEC: our motivation. What are we talking about?

Design and build best in the class inelastic instrument for studying single crystal samples, even small ones, at the Spallation Neutron Source.

➢ Usual constraints of the single crystal studies:

Sample is typically small | *Sample environment is typically bulky.*

1 cent

– *Scattering from the sample environment (cryostat, magnet, furnace, pressure cell, etc) dominates over the sample signal*

– *Polarization analysis is often required to discriminate magnetic signal*

➢ ISIS experience: after more than a decade of operation there is still no instrument which could accept various complex sample environments, or allow polarized beam inelastic studies.

➢ ***Innovative, unorthodox spectrometer design is a key to success***

“Formal” scientific case for the proposed instrument at the SNS.

Neutron spectrometer for studies of the coherent low-energy states in single crystals.

- Coherent collective excitations in single crystals:
  - lattice dynamics (phonons)
  - spin dynamics (magnons, critical scattering)

- Structure and dynamics of partially ordered and glassy states
  - spin glasses
  - charge glasses
  - correlated amorphous phases

- Study of the microscopic physical properties of samples in a variety of extreme environments:
  - magnetic field
  - pressure
  - temperature

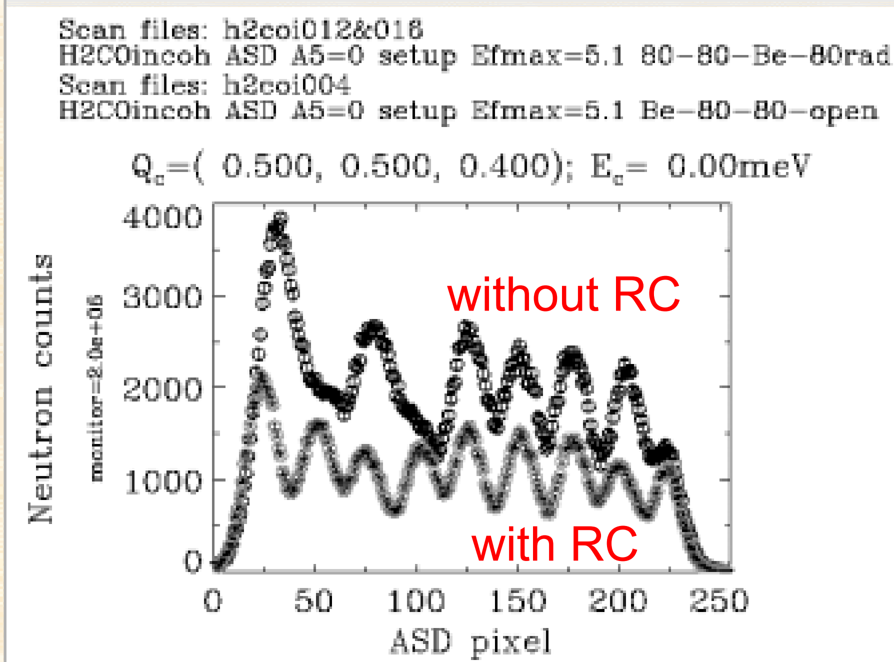
- Characterization of spin-dependent cross-sections by means of polarization analysis

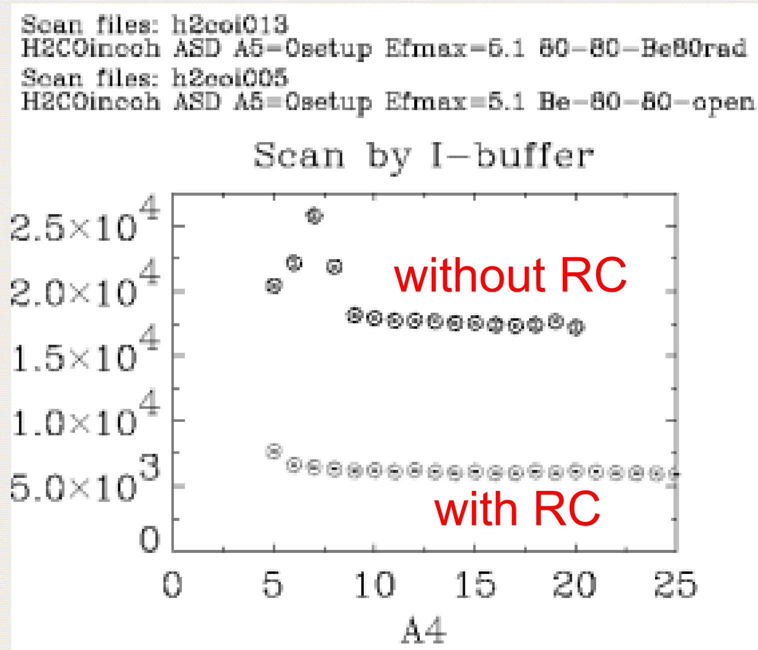
More details and particular examples are given in the Letter of Intent.

HYSPEC: our motivation. How serious the background problem is?

Effect of the radial collimator (RC) in front of the area-sensitive-detector (ASD) in a 3-axis spectrometer SPINS@NCNR.NIST.GOV

Quasielastic background from a standard incoherent scatterer





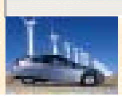
(sample scattering angle)

- *Without RC each ASD pixel views all sample and the analyzer mount*
- *Background increases 2-5 times, disastrously at small scattering angle*
- ***For a background limited measurement (small signal), decrease in background equals to a proportional increase in throughput***

HYSPEC: our motivation. Design objectives.

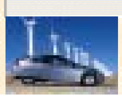
Major unresolved issues in TOF instruments: (i) efficient focusing neutron optics, (ii) polarized beam. Strive for innovation, build on experience.

- ✓ Efficiently use large incident neutron beam by focusing it on the sample
- ✓ Minimize the background: scattering volume seen by a detector should be well defined and easily adjustable
- ✓ Envisage an easy setup of the polarized beam option
- ✓ Optimize the instrument for high throughput at moderate resolution
- ✓ Avoid direct view of the moderator by the sample and its environment
- ✓ Throughput and resolution should be easily traded and vary smoothly over a substantial energy interval, typically from 2.5 meV to 90 meV
- ✓ Both energy and wavevector resolutions should be flexible and easily adjustable, typical resolutions are 1% to 10%
- ✓ Accessible range of scattering angles should be as large as possible



HYSPEC timeline: history of the project.

- January, 2002
  - HYSPEC IDT filed Letter of Intent with SNS
- Fall, 2001
  - Instrument Development Team formed
  - Workshop on the Hybrid Spectrometer held at BNL
  - Refined HYSPEC concept presented to EFAC
- March, 2001
  - Draft proposal of a Direct Geometry Hybrid Spectrometer first presented to EFAC, received positive reply
- December, 2000
  - Completed review of the possible instrument designs
  - Concept of the Hybrid Spectrometer formulated and adopted
- Fall, 1999
  - Center for Neutron Science and Neutron Scattering Group at BNL initiate an effort to design a spectrometer for the SNS



HYSPEC Instrument Development Team and Design Workgroup.

IDT: Current Members and their Institutional Affiliations

I. Zaliznyak, co-PI	BNL
S. M. Shapiro, co-PI	BNL
G. Shirane	BNL
J. Tranquada	BNL
L. Passell	BNL
D. Abernathy	SNS
L. Daemon	Los Alamos
M. Greven	Stanford
B. Gaulin	McMaster
V. Kiryukhin	Rutgers
Y. Lee	MIT
S. Nagler	ORNL
R. Osborn	ANL
J. Rhyne	U. Missouri
C. Stassis	Ames/Iowa St.
A. Zheludev	ORNL

HYSPEC Instrument Design Workgroup

I. Zaliznyak (BNL)

S. M. Shapiro (BNL)

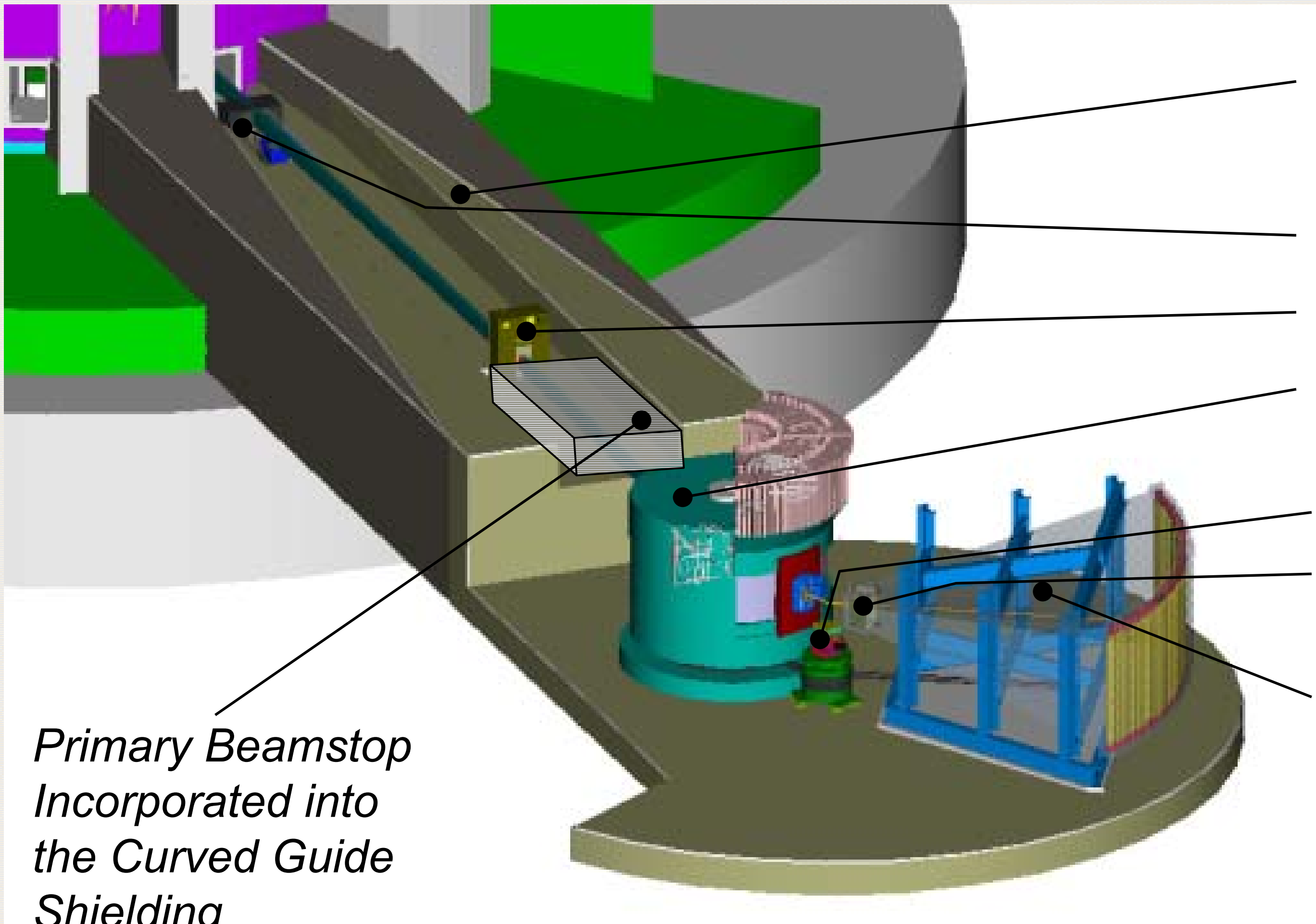
L. Passell (BNL)

V. J. Ghosh (BNL),
Monte-Carlo simulations

S. Doran (SNS/ANL)
Engineering design concept

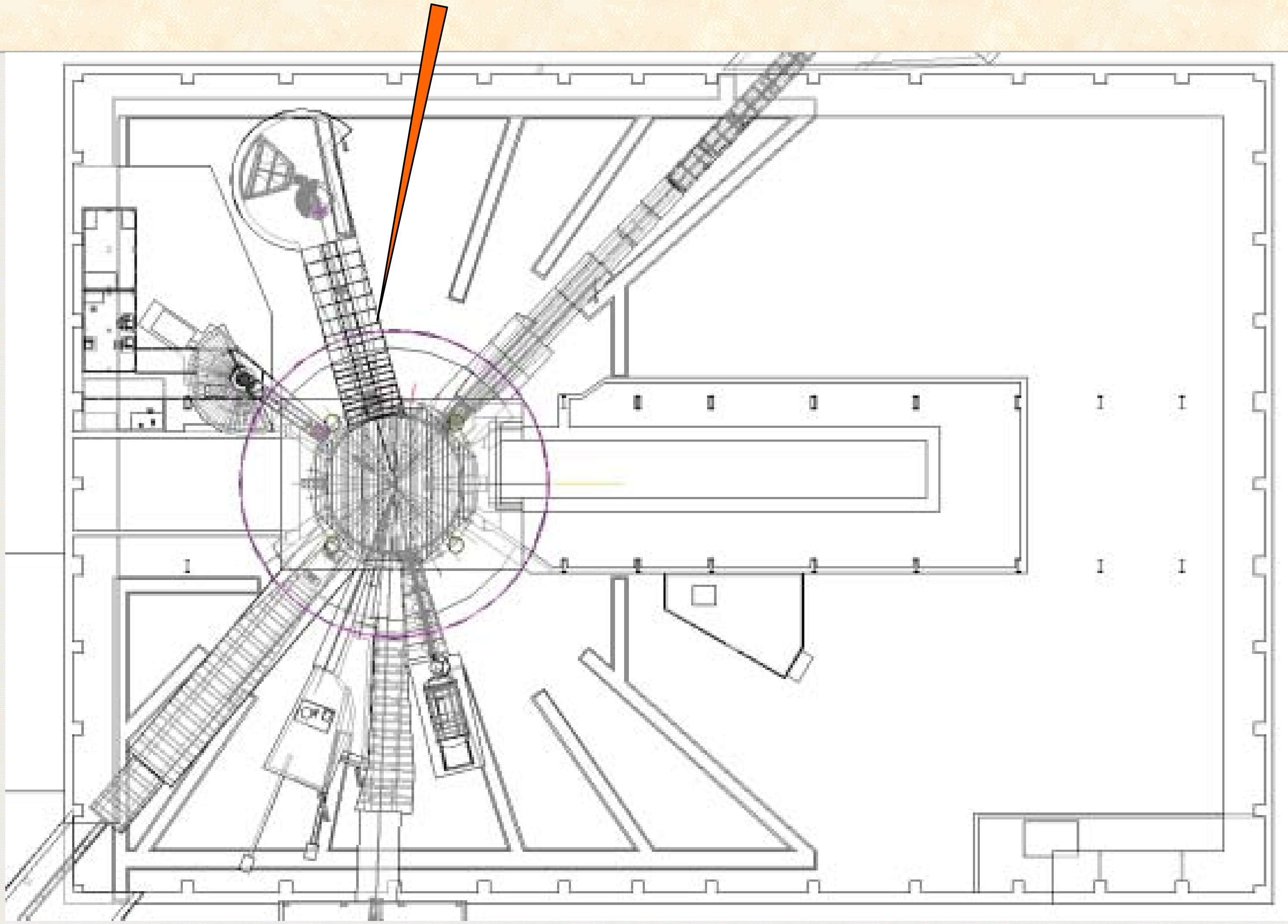
Hybrid Spectrometer BL15 [BNL] conceptual design: layout of main components.

Tentative placement: beamline 15

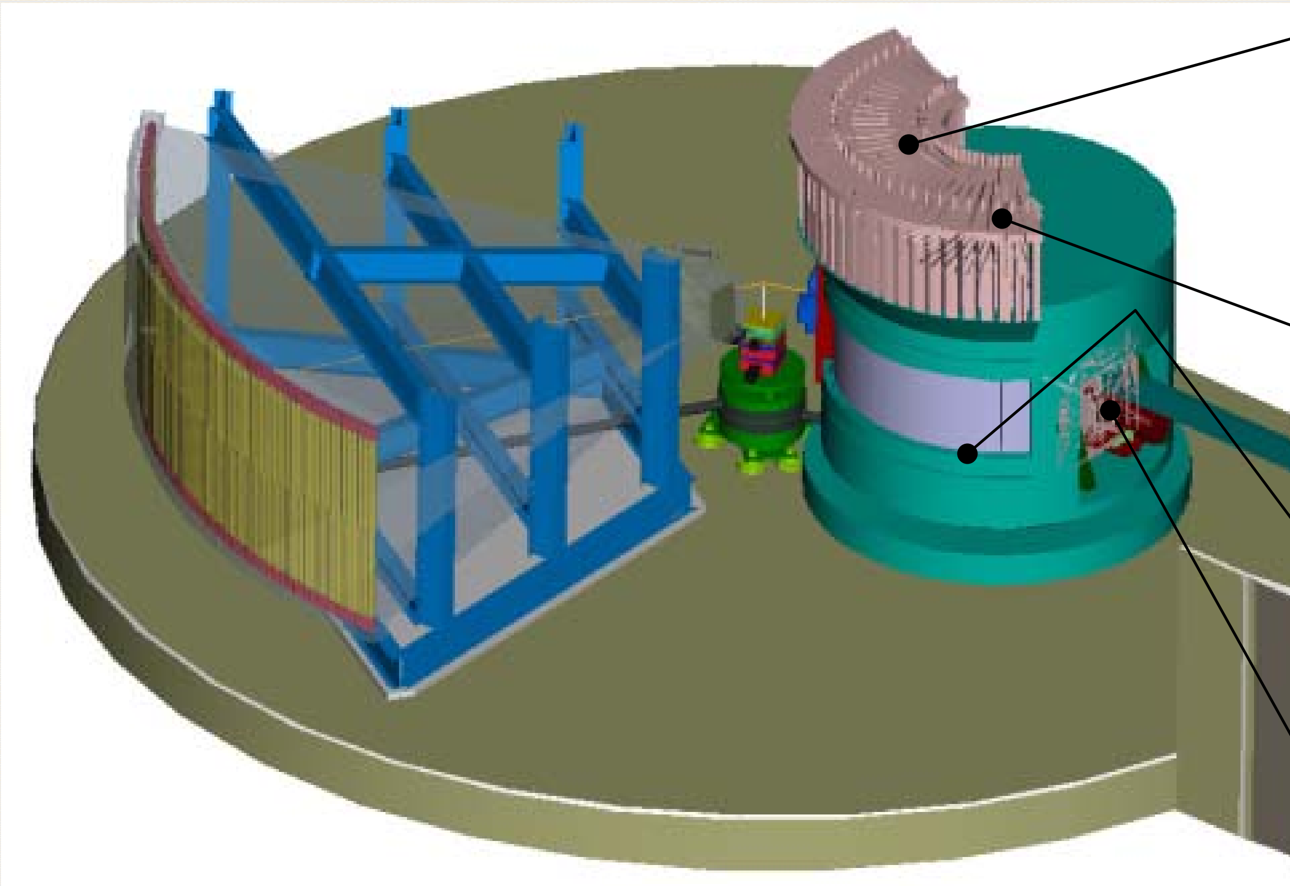


Hybrid Spectrometer BL15 [BNL] conceptual design: floor layout.

Tentative placement: beamline 15



Hybrid Spectrometer BL15 [BNL] conceptual design: setup of the analyzer and experimental area.



Automated Shutter System For Monochrometer

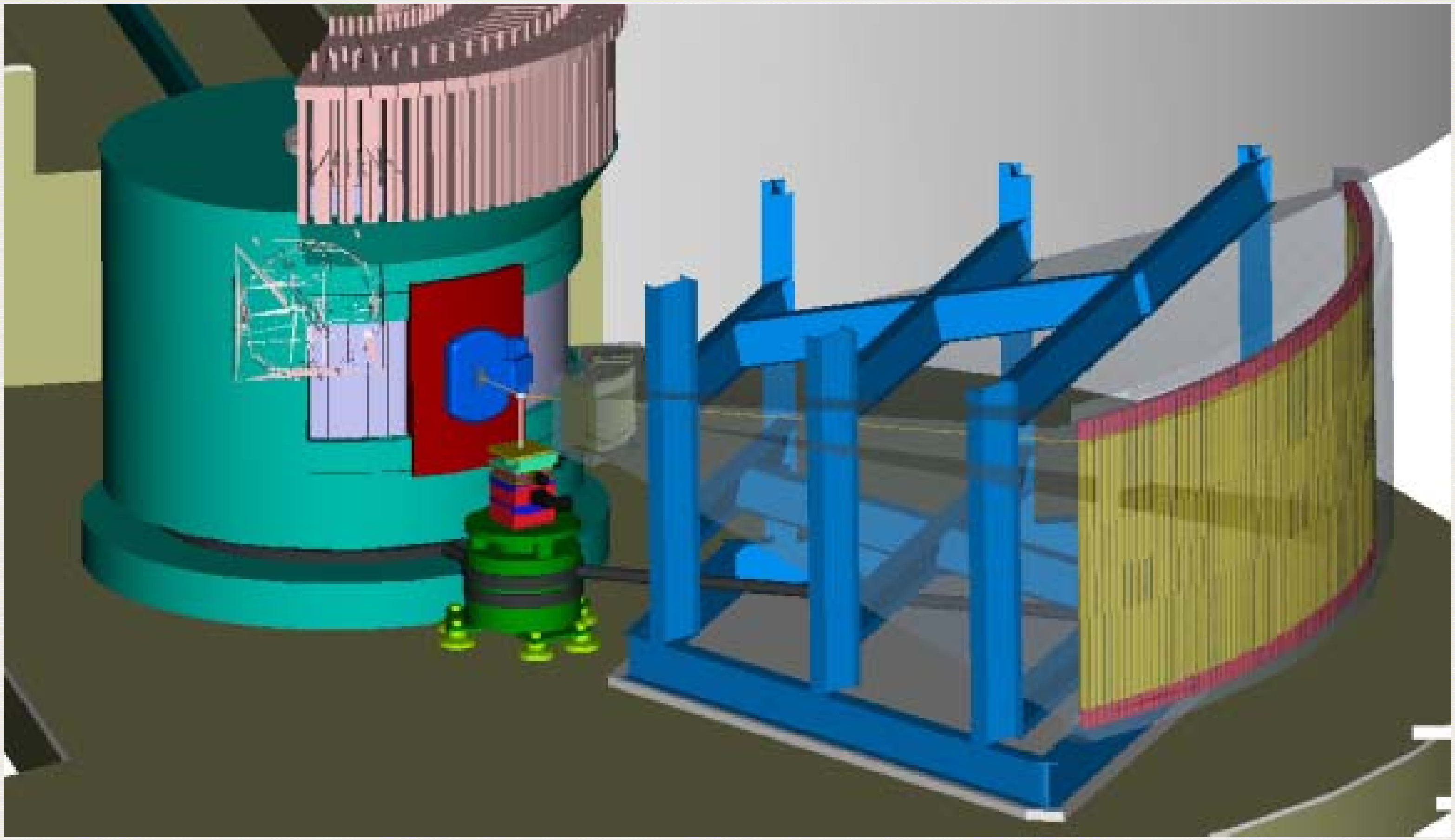
Dual Worm Drive Lifts

Shutters, Each At 5 Degree Increments

Counter Rotating Disk Chopper

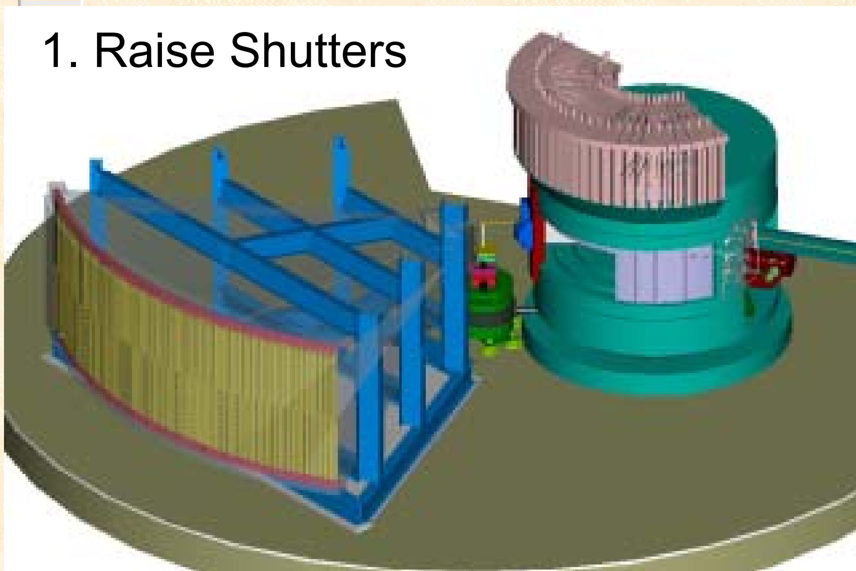
Hybrid Spectrometer BL15 [BNL] conceptual design: typical experimental configuration.

Tentative placement: beamline 15

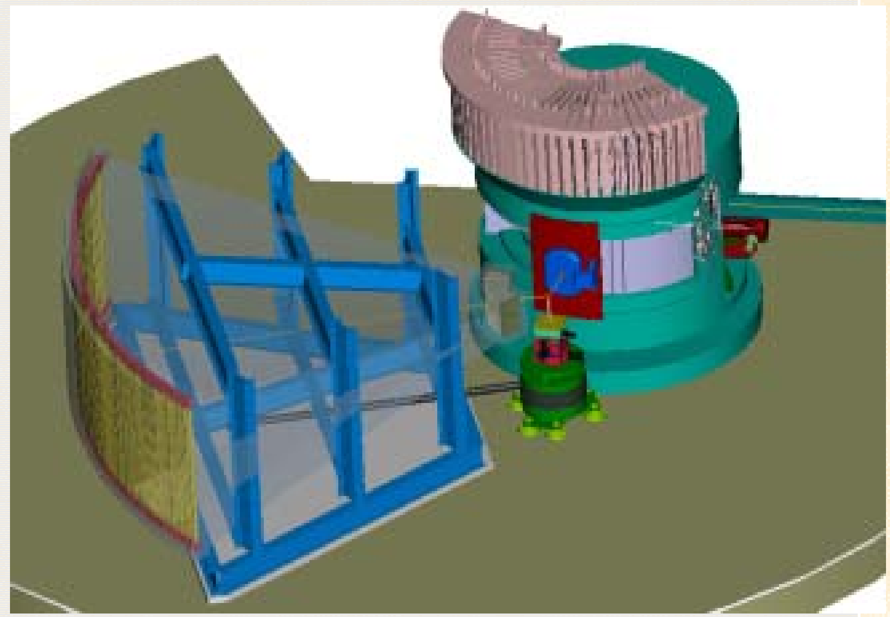


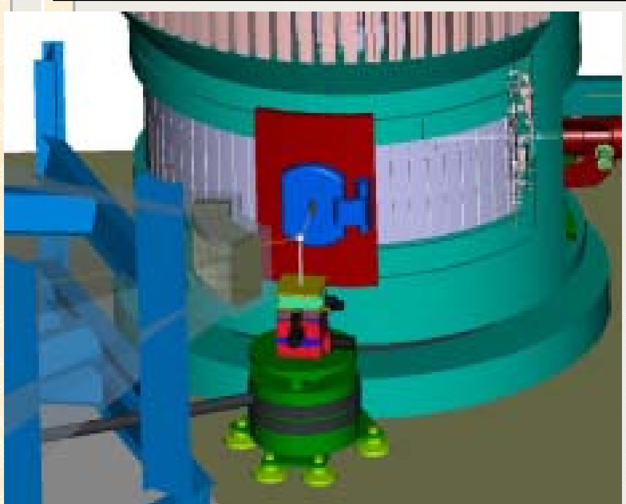
Hybrid Spectrometer BL15 [BNL] conceptual design: some details of the operation.

1. Raise Shutters



2. Swing Sample and Detectors On Airpads

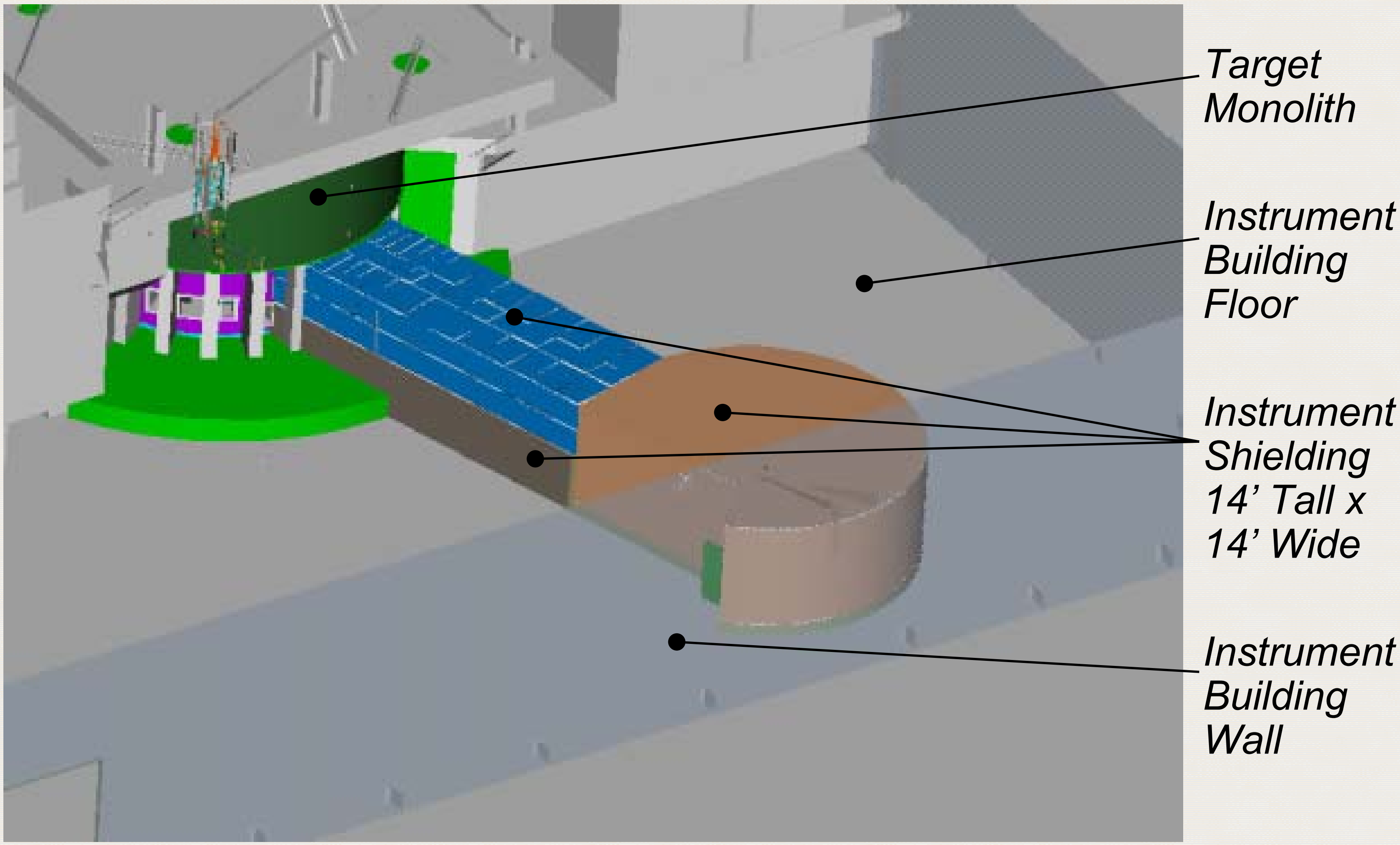




3. Close Shutters

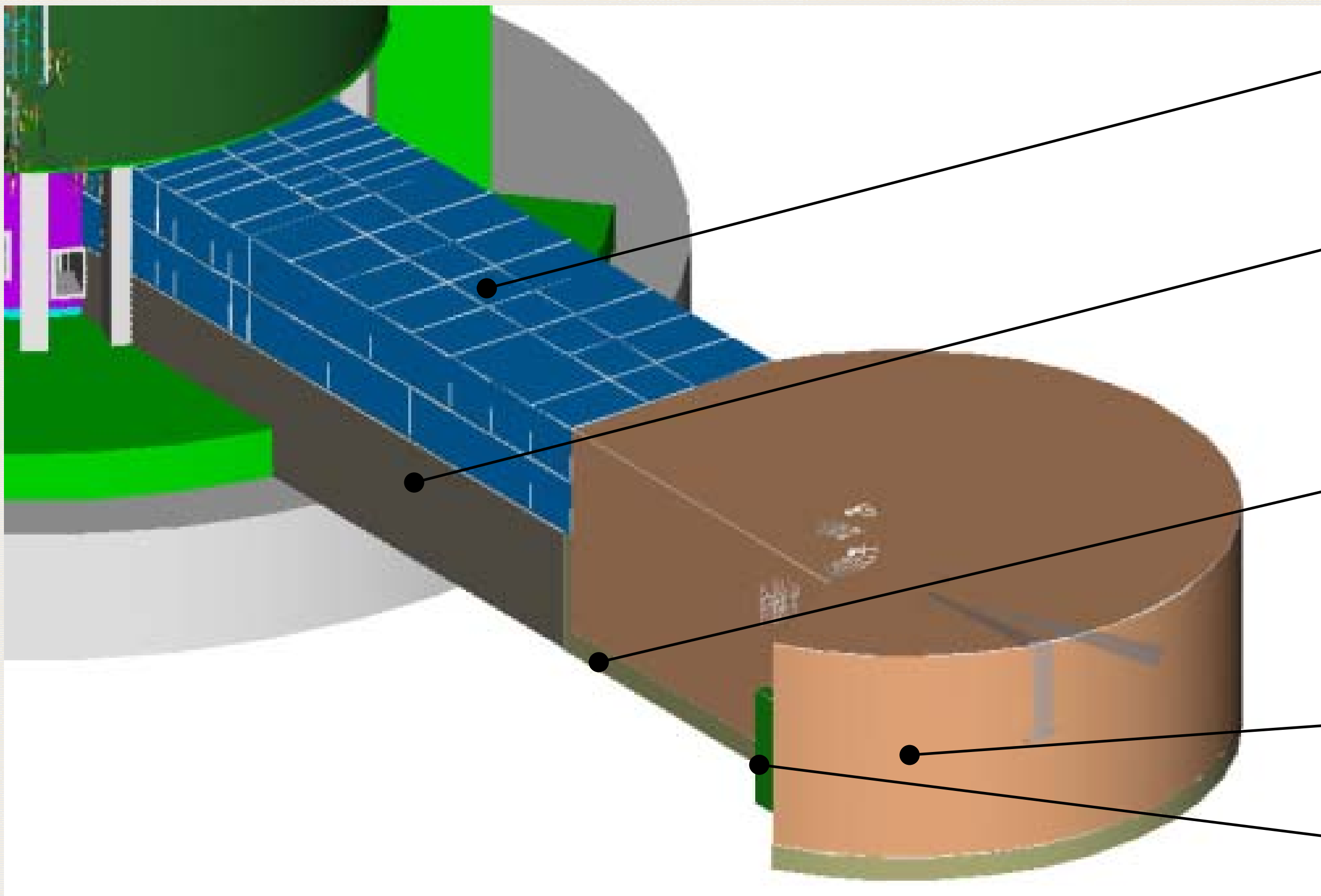
Hybrid Spectrometer BL15 [BNL] conceptual design: general floor layout.

Beamline 15, sample at ~25 m from the moderator, secondary flightpath 4.5 m



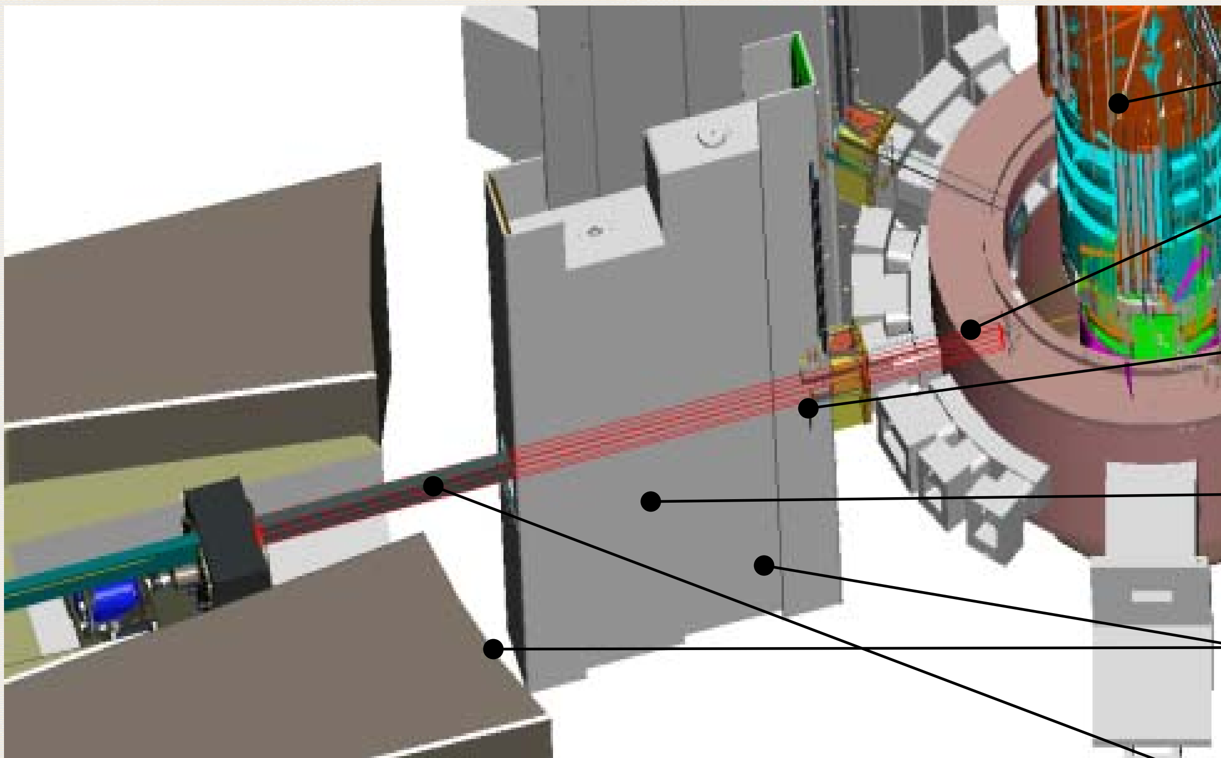
Hybrid Spectrometer BL15 [BNL] conceptual design: shielding.

Tentative placement: beamline 15



Hybrid Spectrometer BL15 [BNL] conceptual design: interface with the moderator.

Tentative placement: beamline 15



Moderator Assembly

Guide 1m from Moderator (highlighted in red)

Core Vessel Insert

Main Beamline Shutter

Shutter Guides

12 cm ->15 cm guide expander

HYSPEC: place in the SNS inelastic instruments suite.

High energy transfer

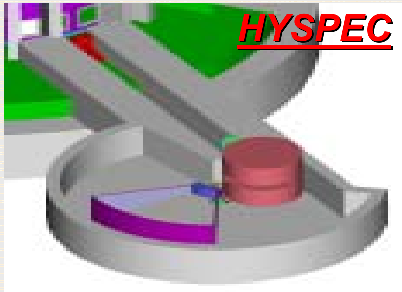
10-1000 meV Fermi Chopper Spectrometer

- E = 10 - 1000 meV
- Q = 0.1 – 22 Å^{-1}

High intensity at moderate resolution and medium energy transfer + polarized beam

Crystal Monochromator Hybrid Spectrometer

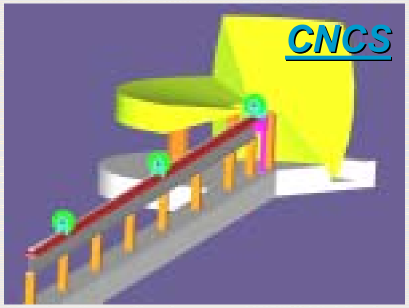
- E = 2.5 - 90 meV
- Q = 0.1 – 8 Å^{-1}



High resolution and low energy transfer

10-100 μeV Multichopper Spectrometer

- E = 2 - 20 meV
- Q = 0.1 - 4 Å^{-1}

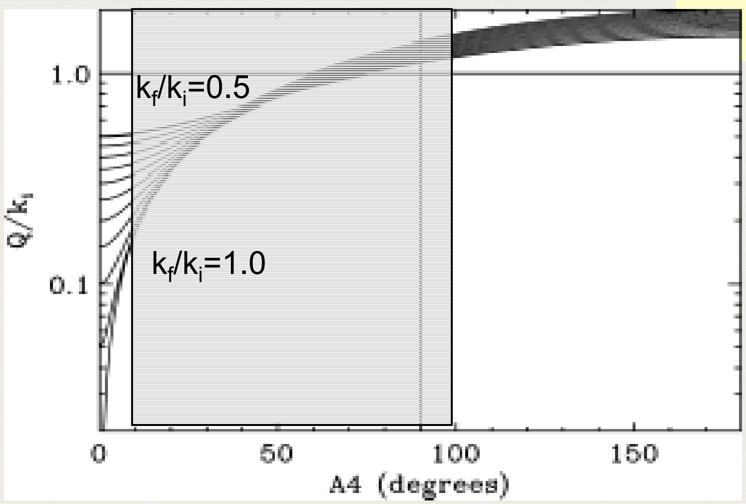


HYSPEC: secondary flight path and analyzer performance.

Uncertainty of the flight time in the analyzer gives largest contribution to the energy resolution.

Analyzer resolution for the length of the secondary flight path L_{SD} = 4 m and L_{SD} = 5 m and for the t=40 μs burst width at the sample (FWHM)

	L_{SD}	Δt/t	ΔE/E
E_f=5.0 meV			
	4 m	0.0098	2.0%
	5 m	0.0078	1.6%
E_f=14.7 meV			
	4 m	0.0168	3.3%
	5 m	0.0134	2.6%
Ef=60.0 meV			
	4 m	0.0339	6.8%
	5 m	0.0271	5.4%



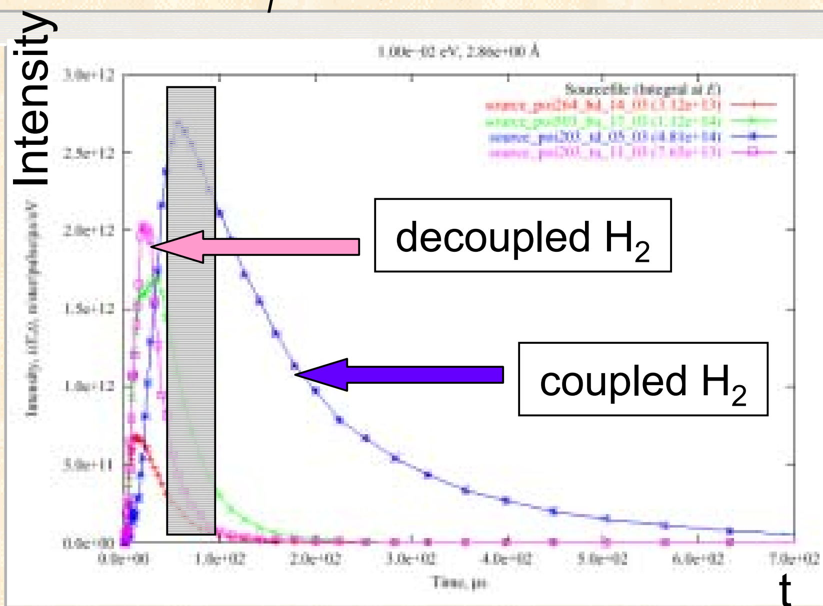
60° - 90° coverage of the scattering angle by the detector array gives simultaneous access to large enough interval in Q for $0.5<k_f/k_i<1$

Moving the analyzer is cost-effective!

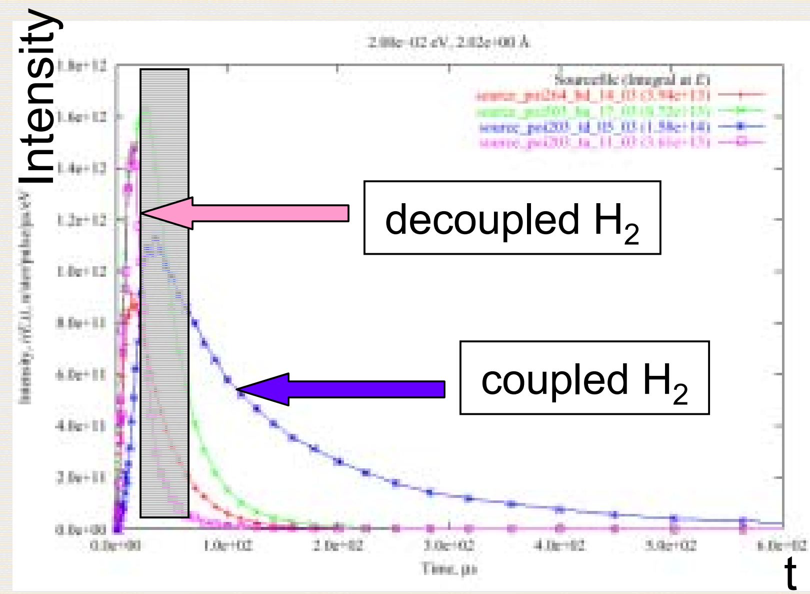
Instrument optimization: choice of the moderator.

"Benchmark" the instrument performance at E_i = 15 meV

E_i = 10 meV



E_i = 20 meV

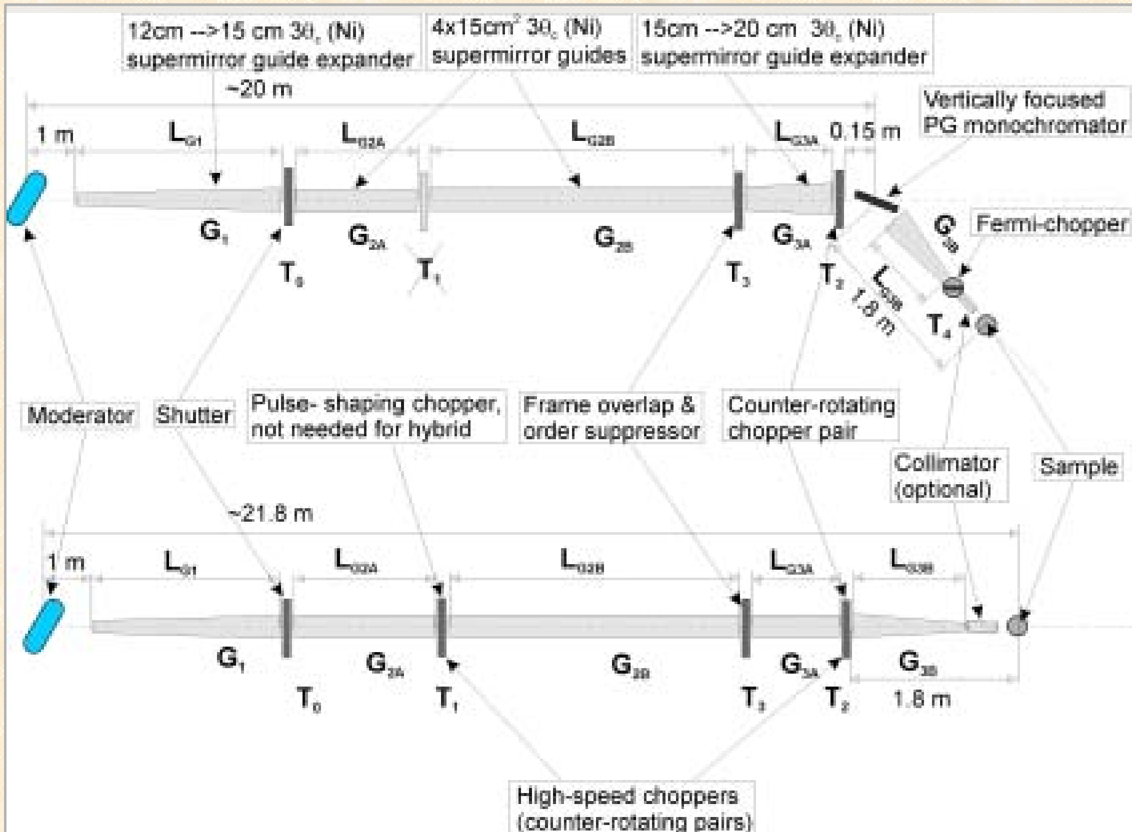


- Figure of merit is the integral flux within 30-50 µs time window, matching the length of the secondary flight-path

Coupled supercritical H_2 moderator

Primary Spectrometers of HYSPEC and a conventional “straight-through” TOF model (MCST) used in Monte-Carlo simulations.

Both setups were optimized for best performance!



	HYBRID MODEL	MCST MODEL
8 c m	G1: 8cm high G2: 8cm high G3A: 8cm G3B: 13.0→5.6cm	G1: 8cm G2A = G2B : 8cm G3A+G3B: 8→2.8cm
1 2 c m	G1: 12cm G2: 12cm G3A: 12cm G3B: 18.0→10.0cm	G1: 12cm G2A=G2B: 12cm G3A+G3B: 12.0→3.4cm
1 5 c m	G1: 12.7→15.0cm G2: 15.0 cm G3A: 15.0→18.0cm G3B: 25.0→10.0cm	G1: 12.7→15.0cm G2A=G2B: 15.0 cm G3A+G3B: 15.0→3.8cm
2 0 c m	G1: 13.8→20.0cm G2: 20.0cm G3A: 20.0cm G3B: 25.0→10.0cm	G1: 13.8→20.0cm G2: 20.0cm G3A+G3B: 20.0→4.6cm

Description of the two models

Coupled Hydrogen moderator 12cm by 12cm

Distance from moderator to sample = 21.8m

All guides are 4cm wide and coated with 3θc supermirror

G2A and G2B are segmented curved guides with an offset of 8cm at T2

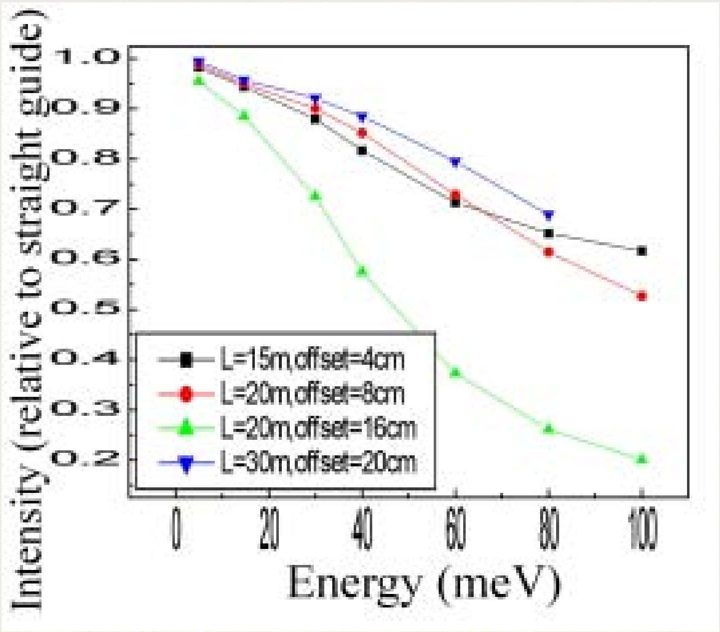
PG vertical mosaic = 0.4°, horizontal mosaic = 1.0°

Distance between collimator and sample is 40cm

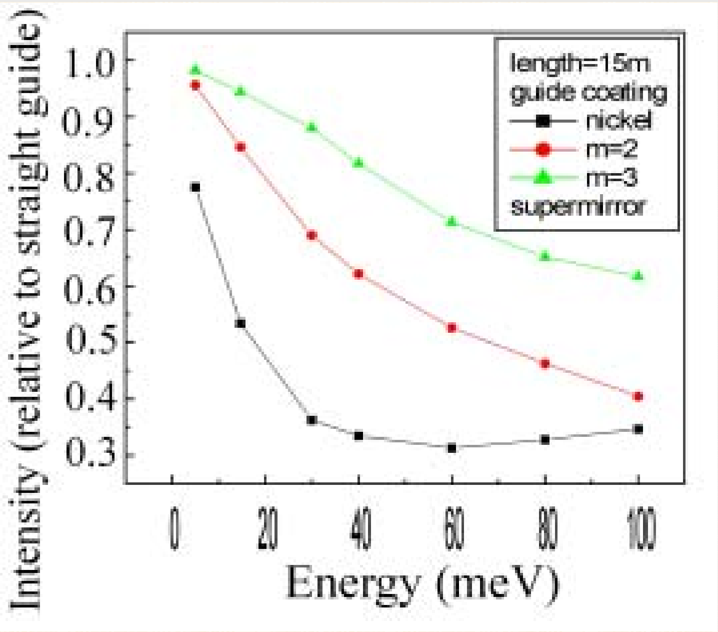
The side view of the guide cross-section is shown schematically

Performance of the guide.

Impact of the guide curvature (relative to the similar straight guide)



Impact of the guide coating (relative to $3\theta_c$ supermirror guide)

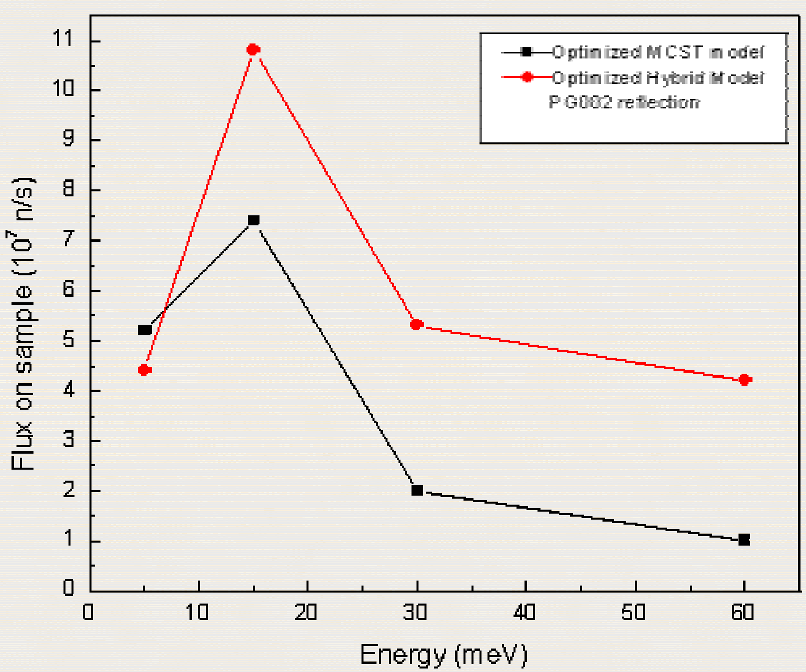


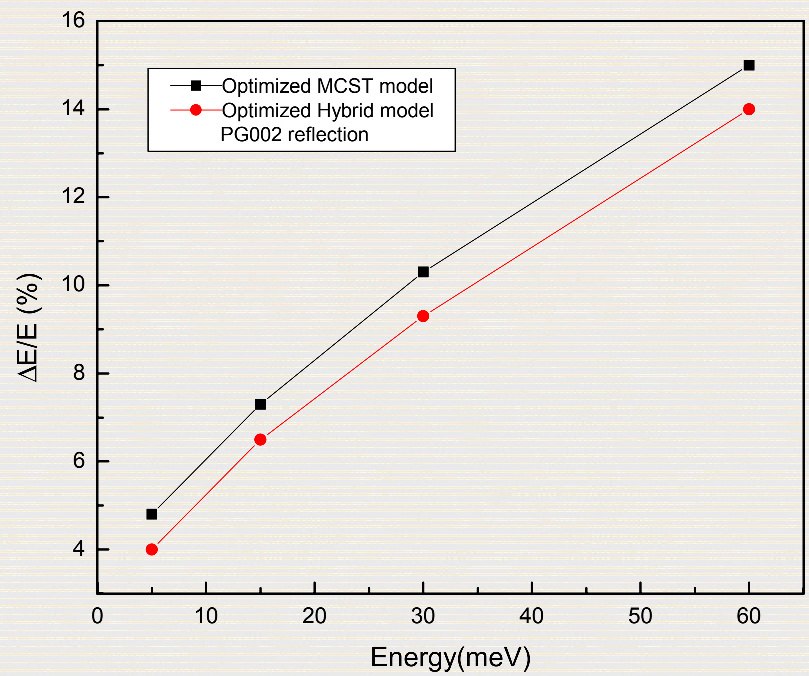
- L = 20 m curved $3\theta_c$ supermirror guide at a reasonable offset of 8 cm ~ 2 times the width of the guide provides ~75% transmission at 60 meV
- Offset of 12 cm may still be OK, especially for a longer (L~25 m) guide

Flux on sample and energy resolution for two models obtained from MC simulation using NISP package.

HYSPEC vs MCST: neutron current through a 2x2 cm^2 sample

HYSPEC vs MCST: monochromator energy resolution (FWHM)



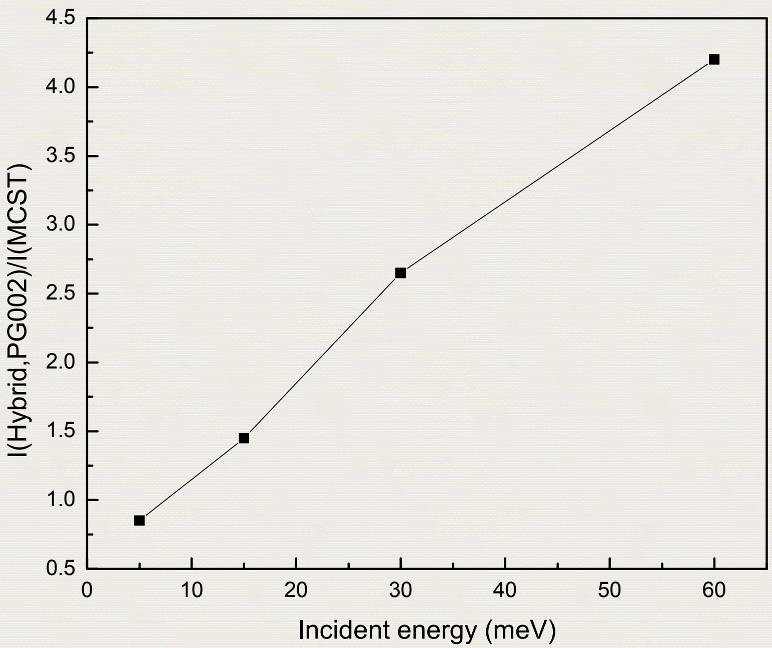


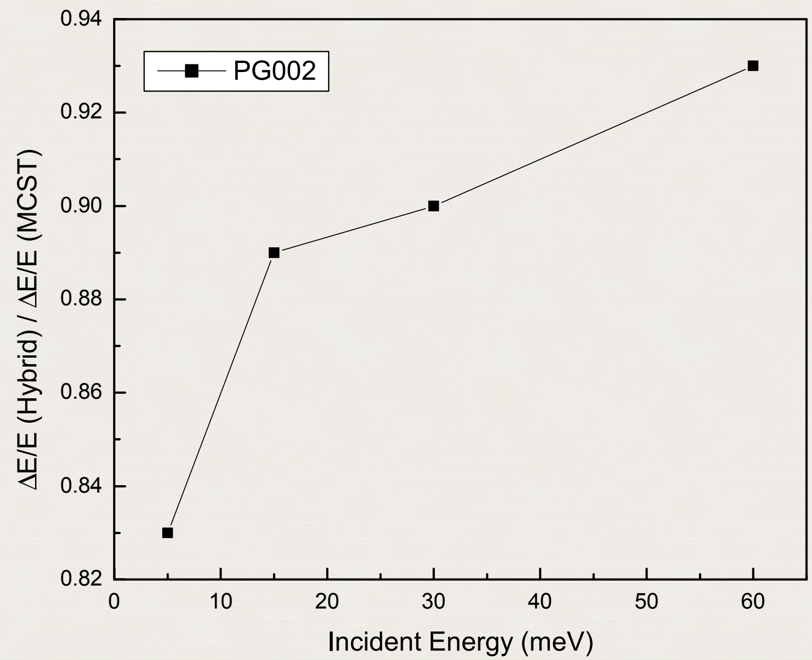
- *Decrease in intensity for hybrid spectrometer at E_i<10 meV is because of the better energy resolution*
- ***Focusing monochromator yields a gain of factor 2 to 5 for Ei>15meV!***

Relative flux on sample and energy resolution for two models obtained from MC simulation using NISP package.

Ratio of the neutron flux on a 2x2 cm^2 sample for HYSPEC and MCST

Ratio of the monochromator energy resolutions for HYSPEC and MCST

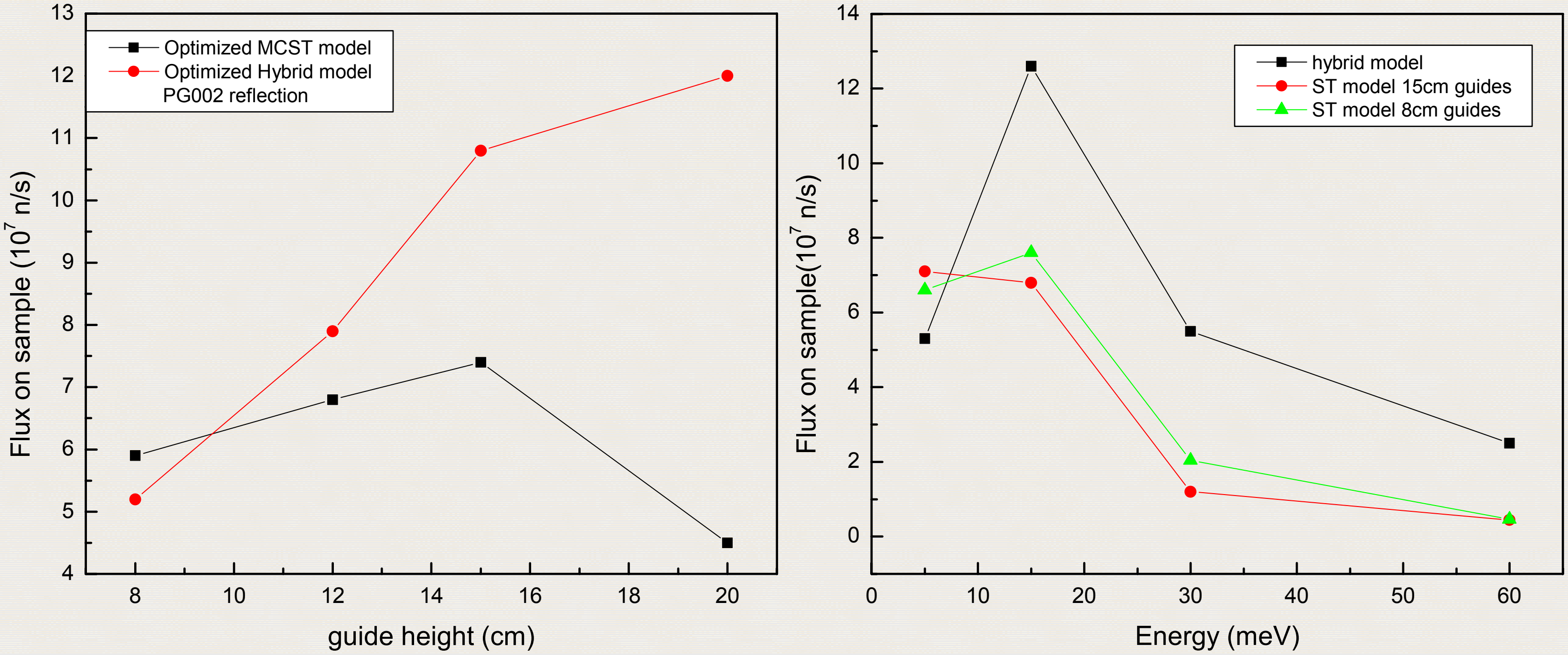




- *Smaller intensity for hybrid spectrometer at E_i<5 meV is because of the better energy resolution*
- ***Focusing monochromator yields a gain of factor 2 to 5 for Ei>15meV!***

Hybrid spectrometer: where does the gain come from?

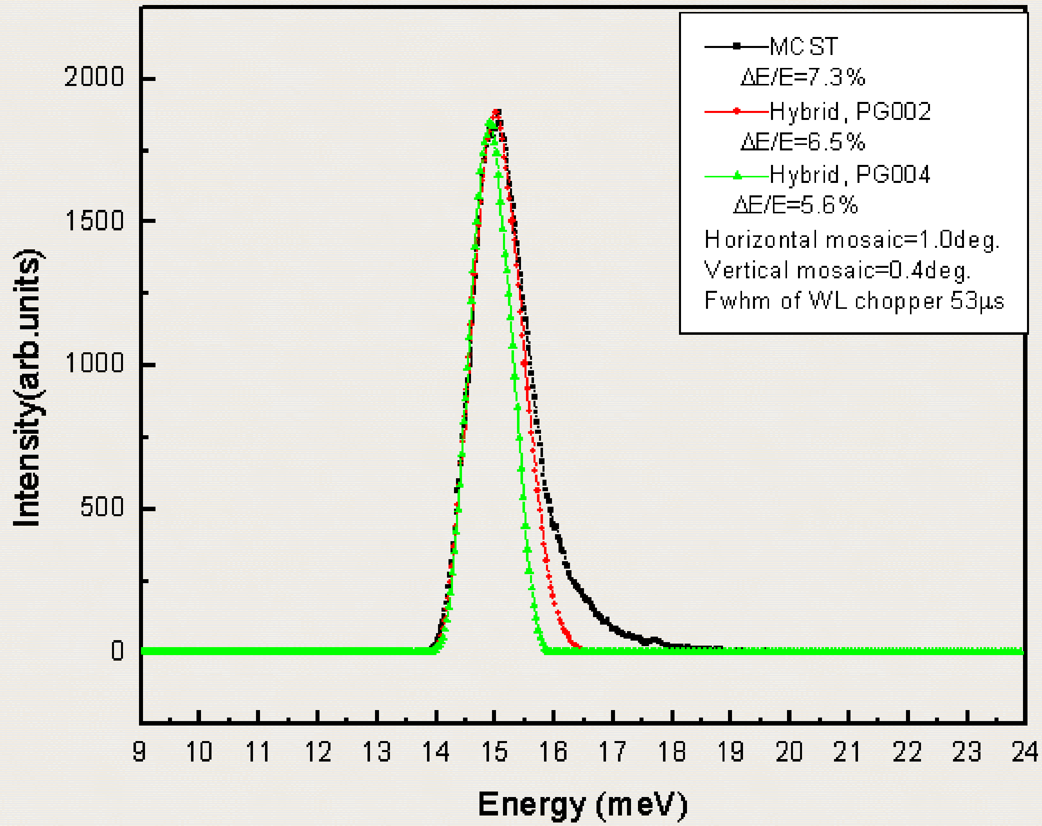
Efficient use of the tall guide



➢ *Relative performance of the hybrid instrument at lower energies will improve further if more realistic m=2 guide coating is implied*

HYSPEC: resolution function for the elastic scattering.

HYSPEC versus MCST: energy resolution function for elastic scattering at E_i=15 meV, normalized to the same height

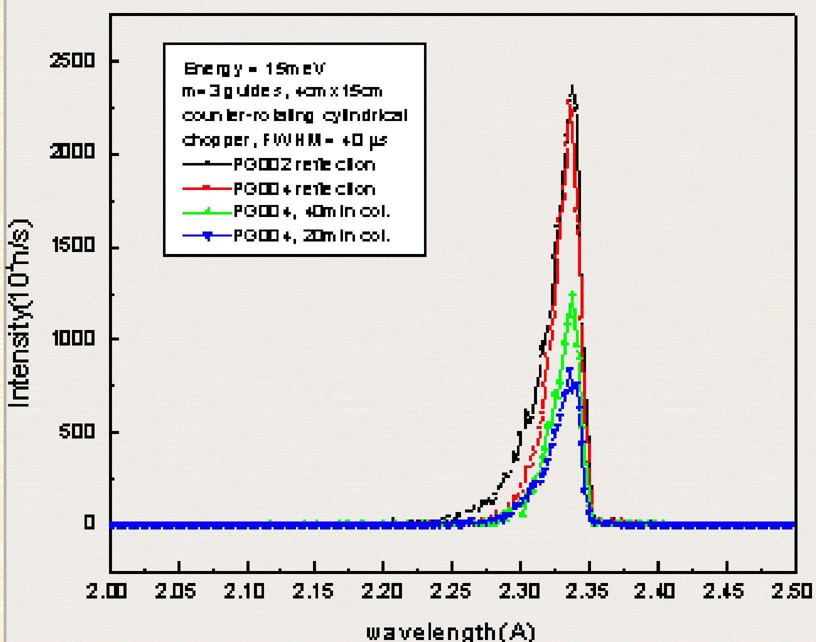


- *High-E tail is nicely cut by the monochromator, especially PG(004)*
- *Relative performance of HYSPEC will improve further by about 20% if only the useful neutrons within the resolution FWHM are counted*

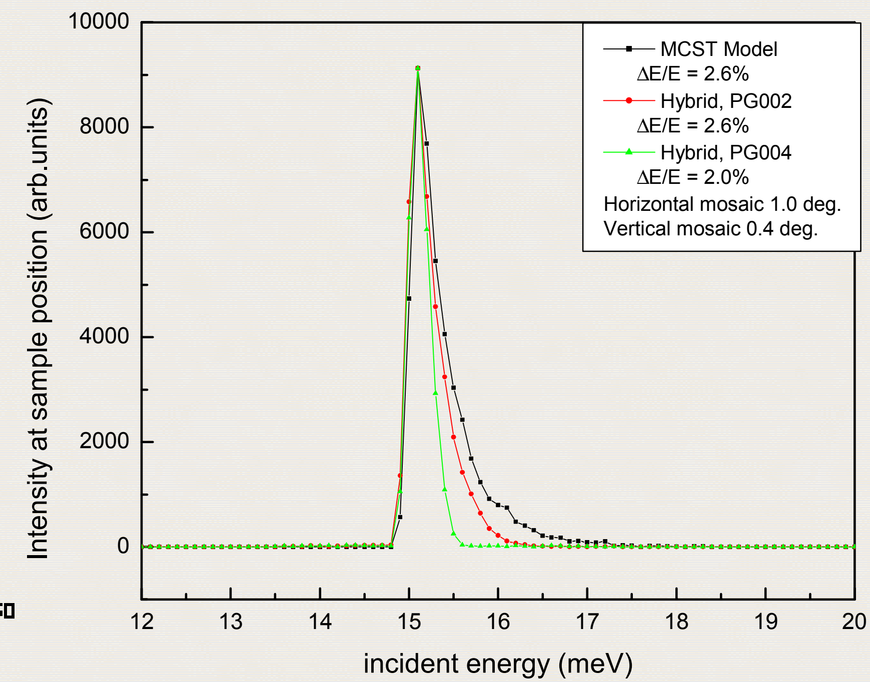
HYSPEC: monochromator resolution function.

High-E tail is nicely cut by the monochromator, especially PG(004)

<u>HYSPEC</u>: wavelength distribution of neutrons incident on the sample for different PG reflections and collimation

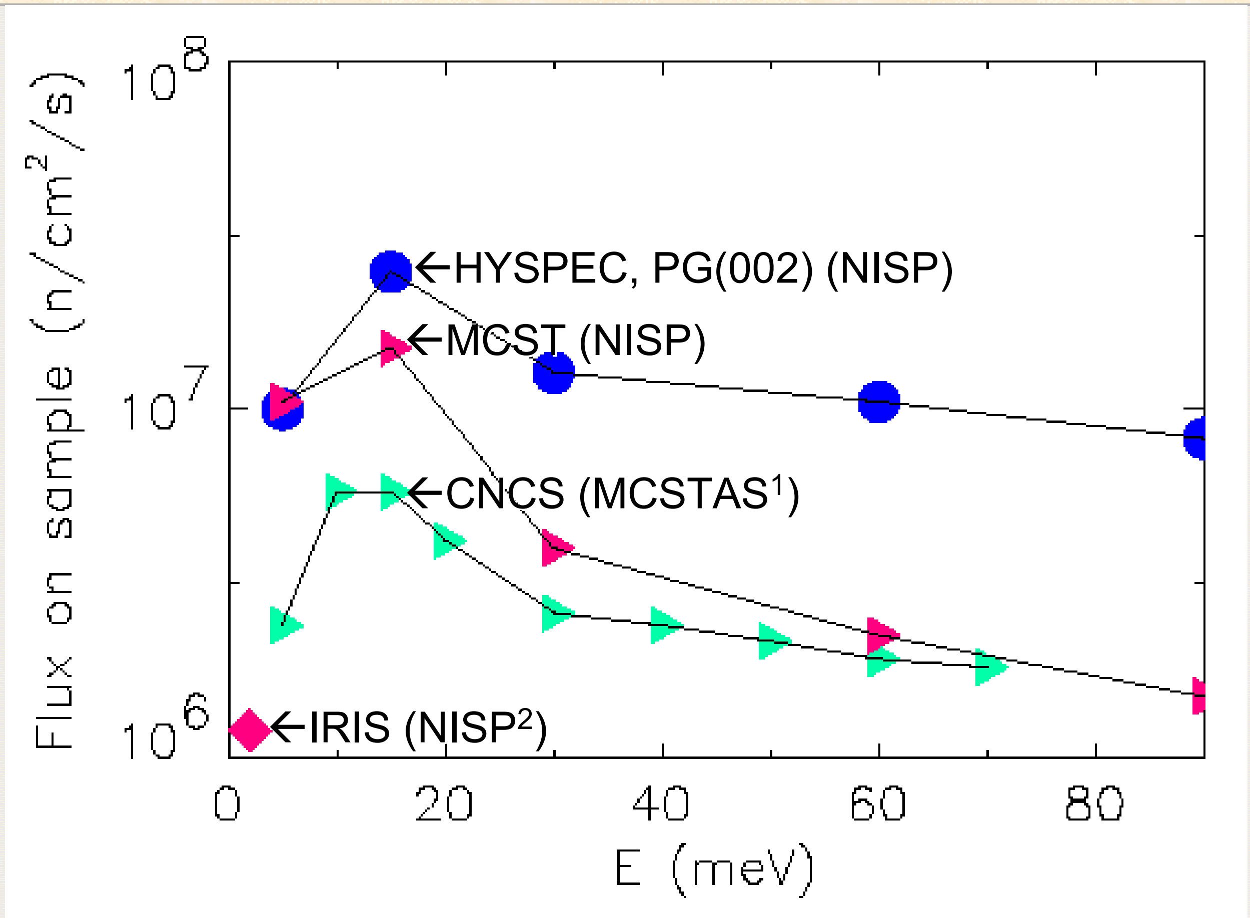


<u>HYSPEC versus MCST</u>: incident energy distributions normalized to the same height



- *Relative performance of HYSPEC will improve further by about 20% if only the useful neutrons within the resolution FWHM are counted*

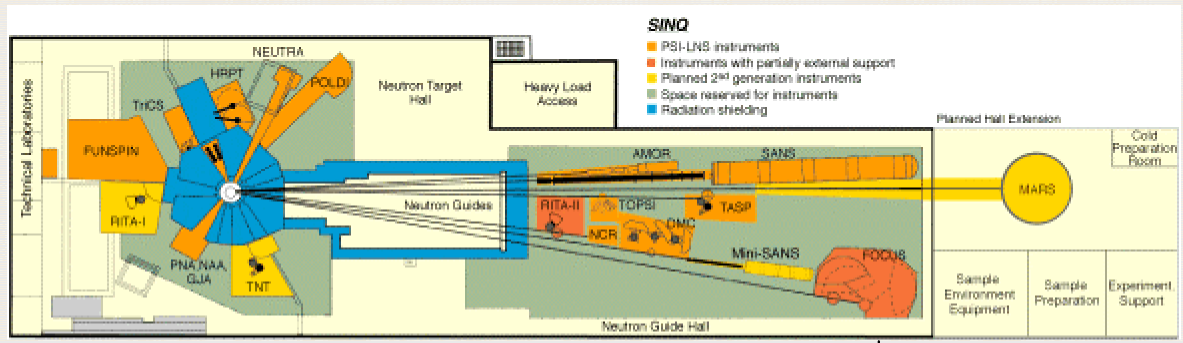
Calculated flux on the sample: HYSPEC, MCST, CNCS and IRIS



[1]MCSTAS data for CNCS are by G. Granroth (2001), normalized to 64 μs burst time
[2]NISP simulation for IRIS by V. Ghosh, normalized to 4% E-resolution

Operational prototype: direct geometry hybrid spectrometer FOCUS@SINQ.PSI.CH. “Off-the-shelf” system?

Layout of the SINQ experimental hall



FOCUS spectrometer

Operational prototype: schematics of the FOCUS concept, mode of operation and technical details.

Concept so attractive, they even chop a CONTINUOUS beam!

356 S. Janssen et al. / Physica B 283 (2000) 355–360

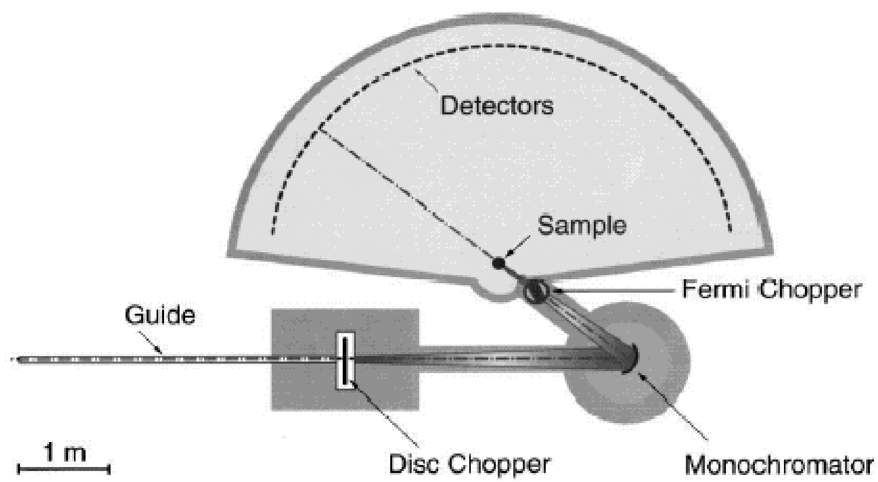


Fig. 1. Schematic layout of SINQ's cold neutron time-of-flight spectrometer FOCUS. The instrument combines a double-focusing crystal monochromator, a Fermi chopper, and a disc chopper.

FOCUS setting	Rel. intensity	ν_{Fermi} (Hz)	Neutron Energy Loss [meV]			
			0.0 (elastic peak) ΔE [meV]	8.7 ΔE [meV]	10.2 ΔE [meV]	10.9 ΔE [meV]
TF 002	1.00	42	3.027 ± 0.057	1.023 ± 0.009	0.982 ± 0.017	0.658 ± 0.012
TF 004	0.31	107	1.245 ± 0.008	0.584 ± 0.019	0.423 ± 0.015	0.428 ± 0.011
MF 002	0.14 (0.28)	333	0.690 ± 0.012	0.607 ± 0.035	0.545 ± 0.056	0.612 ± 0.064
MF 004	0.07 (0.14)	333	0.544 ± 0.013	0.382 ± 0.030	0.272 ± 0.035	0.301 ± 0.032

Operational prototype: FOCUS technical characteristics and first results.

S. Janssen et al. Physica B 283 (2000)

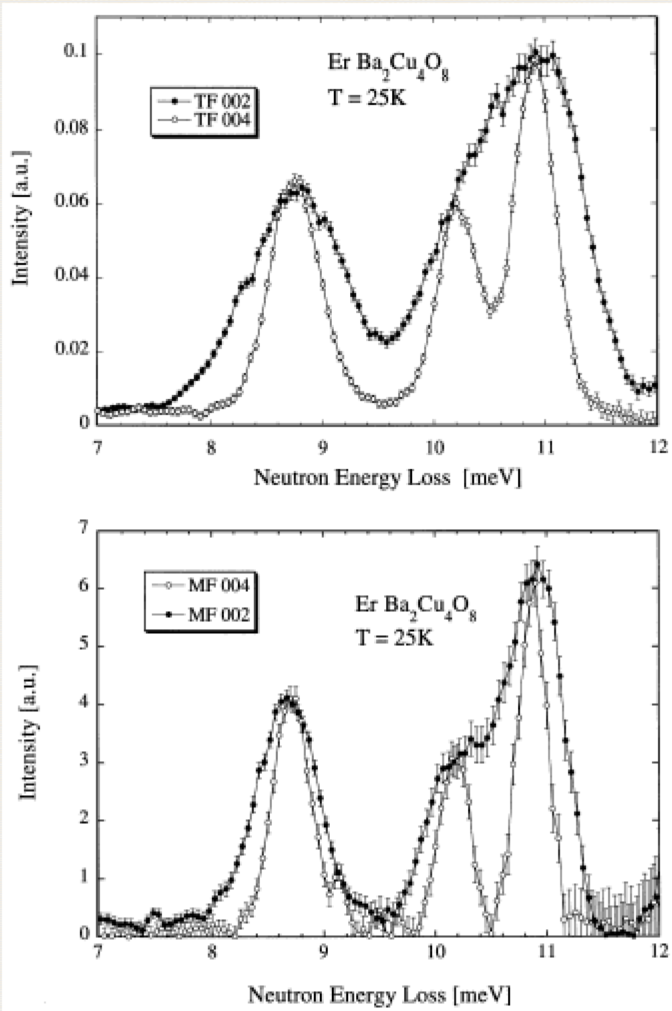
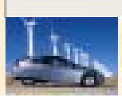


Fig. 4. Crystal electric field spectroscopy on $ErBa_2Cu_4O_8$ at $T = 25$ K obtained on FOCUS using either a TF (upper part) or a MF (lower part) setup of the instrument. The PG 002 (full symbols) as well as the 004 reflection (open symbols) were used.

Monochromator	Bragg angle	E_i [meV]	Res_{elast} [meV]	Q_{max}[Å]
PG002	17.5	20.0	1.00	5.6
PG002	36.6	5.1	0.14	2.8
PG002	63.4	2.3	0.04	1.9
PG004	36.6	20.0	0.50	5.6
Mica 002	65.4	0.3	0.01	0.6



HYSPEC vs FOCUS : what is the difference?

Most important: pulsed beam allows using up to ~1/2 of the total amount of neutrons produced => gain factor ~100

HYSPEC:

- *monochromator with vertical focusing immediately follows the guide, at <1.8 m from the sample*
- *longer, 4.5 m secondary flightpath*
- *thick PG crystals with anisotropic mosaic*
- *Heusler crystal monochromator for polarized beam*
- *guide tube before sample*

➢ ***HYSPEC will do better***

Summary of the technical features of a proposed direct geometry hybrid instrument for the SNS.

Tall neutron guide + efficient vertical focusing provide excellent data collection rate, allowing studies of very small samples in challenging environments

- Resolution: dE/E~0.03-0.1, dQ/Q~0.01-0.03

- High flexibility
  - continuous variation of the incident energy from 2.5 to 90 meV with no higher-order contamination
  - full range of energy transfers available at each Q
  - easily and broadly variable energy and Q resolution
  - possibility of time focusing/defocusing
  - easily adaptable for polarization analysis

- Low-background and friendly to demanding sample environment
  - standard sample table accepts many different sample environments
  - sample is away from the direct beam
  - scattering volume is well defined by collimators and slits

- High sensitivity to small scattering cross-sections (signal to BG ratio)

- Can be operated at small scattering angles (near the forward direction)

Summary of the principal features of the proposed hybrid spectrometer (how do we fit our wish list?) .

Bonus: *monochromator shapes resolution function, cutting ugly high-E tail.*

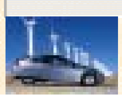
- ***High flux on sample at E_i = 5 - 90 meV:*** *tall neutron guide + efficient vertical focusing by curved crystal monochromator.*

- ***Polarized beam option:*** *polarized incident neutron beam for E_i = 5 - 90 meV, polarization analysis of the scattered beam for E_f < 15 meV.*

- ***Low background with bulky sample environments:*** *collimator(s)+slit(s) define scattering volume seen by detector(s) and restrict analyzer acceptance to scattering from sample only. Scattering from cryogenic environment, magnet, pressure cell, etc., is mostly rejected.*

- ***Continuous wavevector coverage:*** *no "blind spots" caused by spaces in the detector array.*

- ***Flexibility:*** *both energy and wavevector resolutions are variable and easily adjustable, typical resolutions are 1% to 10%. In addition, different crystal reflections may be user on monochromator.*



Current issues and future plans.

Current issues

- *EFAC evaluation of the proposed spectrometer*
- *Main beam stop and beamline shielding simulations*
- *Mobile "sloppy Fermi-chopper" design for high-E-resolution operation (alternative/additional T_2 chopper, placed after the monochromator)*

Future plans

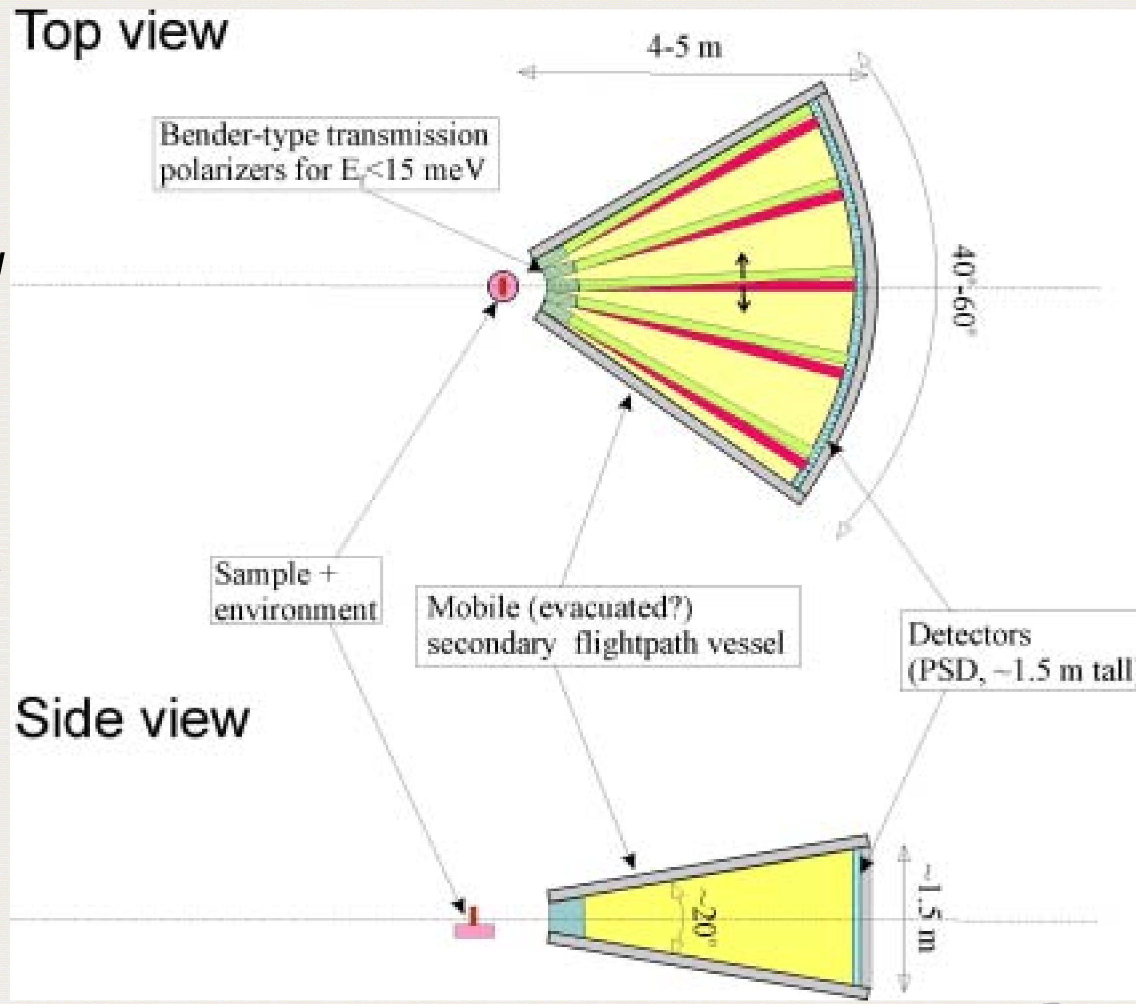
- *Get more seed funding to put together a cost estimate based on a realistic designs of the spectrometer components*
- *Put together a comprehensive proposal and search for funding.*
- *Work on further optimization of the instrument setup.*

APPENDIX. Secondary spectrometer (TOF analyzer) and its operation in the polarized beam mode.

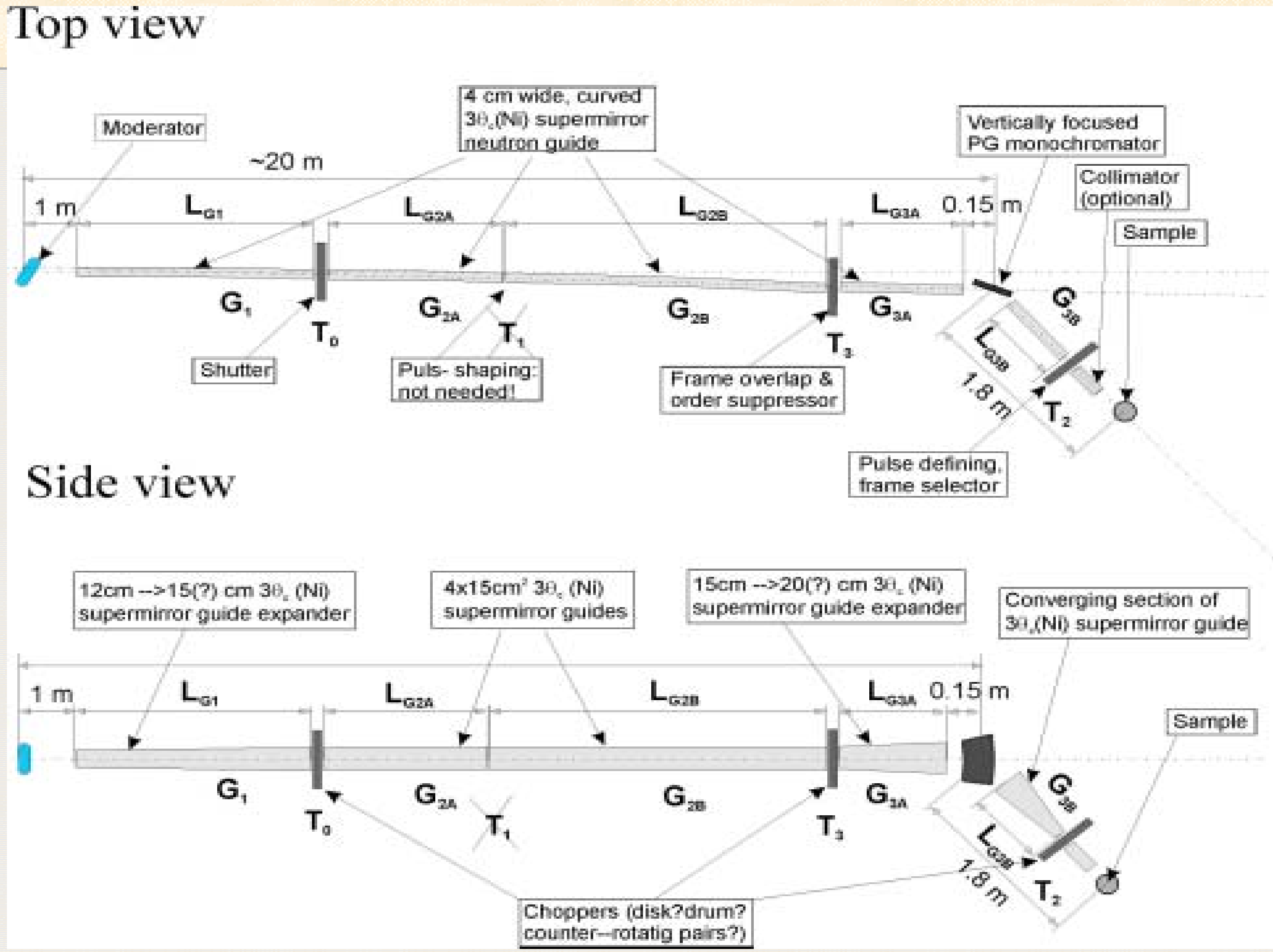
All scattering angles of interest in the polarized mode are filled in by appropriately moving the detector bank

- *E_i=5-90 meV incident polarized beam is produced by reflection from VF Heusler crystal monochromator*
- *Set of 5-10 bender-type polarizers provide for the polarization analysis for E_f<15 meV.*

- *Scattering from the BULKY SAMPLE ENVIRONMENT (aluminium, etc.) is outside analyzer acceptance.*



APPENDIX. Schematics of the proposed primary spectrometer.



APPENDIX. Pro’s and Con’s of a Crystal Monochromator.

Advantages of a crystal monochromator

- beam may be compressed on the sample using focusing Bragg optics, beam height is not limited
- sample and its environment are exposed to reflected monochromatic beam only: reduced background
- works for wide beams
- resolution is easily adjusted by putting the collimators
- (Heusler) may provide a polarized beam for energies up to ~60 meV

Disadvantages of a crystal monochromator

- lower than one and energy-dependent reflectivity of the crystal, is not well-suited for providing high-energy incident neutrons
- energy and wavevector resolutions are coupled and depend on the instrument position
- sample table and secondary spectrometer need to be moved when incident neutrons energy is changed