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

Neutron Scattering Group

BROOKHAVEN NATIONAL LABORATORY

- **Igor Zaliznyak**
- **Laurence Passell**

BROOKHAVEN NATIONAL LABORATORY

Outline

- ❑ *Scientific case and design objectives for the proposed hybrid spectrometer for the SNS*
- ❑ *General layout of the proposed spectrometer and its place in the SNS instrument suite*
- ❑ *Comparison of different spectrometer concepts and evolution of our thinking*
- ❑ *Preliminary analysis of the instrument performance*

Scientific case for a proposed instrument for 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)

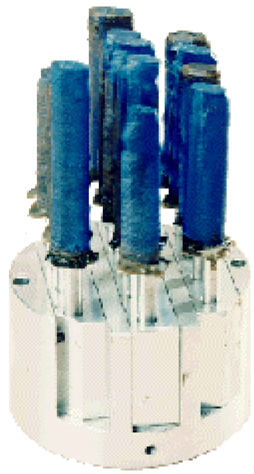
- Structure and dynamics of partially ordered and glassy states
  - spin glasses
  - charge glasses
  - correlated amorphous phases

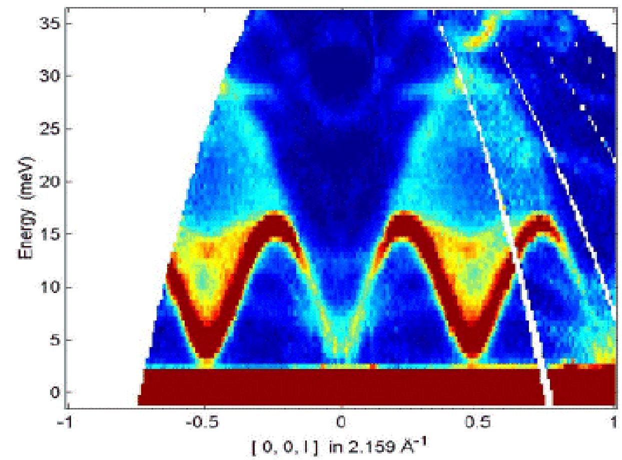
- Study of the microscopic physical properties of samples in a variety of extreme environments:
  - magnetic field
  - pressure
  - temperature

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

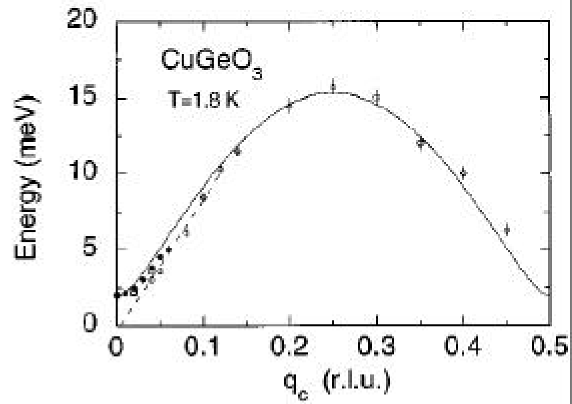
What are the typical samples we want to study?

$CuGeO_3$ sample used by M. Arai group for detailed measurement of the excitation dispersion on MAPS in 2000





$CuGeO_3$ sample used by L.-P. Regnault for the original measurement in 1993



Benchmark requirements for a single crystal neutron spectrometer

- Transmission of both primary (monochromator) and secondary (analyzer) spectrometers should be close to 1 within the resolution acceptance range, and vary smoothly over a substantial energy interval, typically from 2.5 meV to 60 meV.

- Both spectral (energy resolution) and angular (~ wavevector resolution) acceptances of the monochromator and analyzer should be flexible and easily adjustable, typical resolutions are 1% to 5%.

- Scattering volume seen by a detector should be well defined and easily adjustable depending on the sample size to minimize the background.

- Efficient use of the large incident neutron beam by focusing it on the sample is very important, and should be previewed.

What are our main design goals?

- Use most of the monochromatic neutron intensity produced by the source, while providing the highest possible signal-to-background ratio in the detector at a good to moderate energy and wavevector resolution

- Use the pulsed time structure of the neutron beam at the SNS
- Avoid the direct view of the moderator and the source by the sample
- Make solid angle accepted by the secondary spectrometer as large as necessary
- Make range of the scattering angles accessible to the secondary spectrometer as large as possible
- Preview an easy setup of the polarized beam option
- Trade-off of the resolution for intensity should not degrade the instrument performance

How does the instrument we propose fit SNS inelastic instruments suite?

High energy transfer

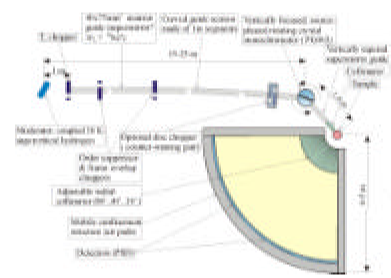
10-1000 meV Fermi Chopper Spectrometer

- 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

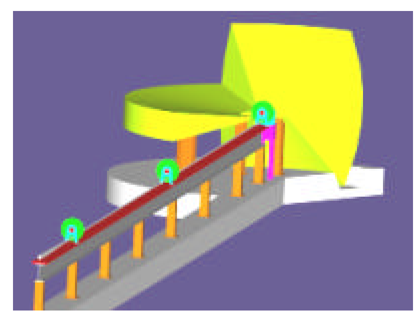
- E = 2.5 - 60 meV
- Q = 0.1 – 8 Å^{-1}



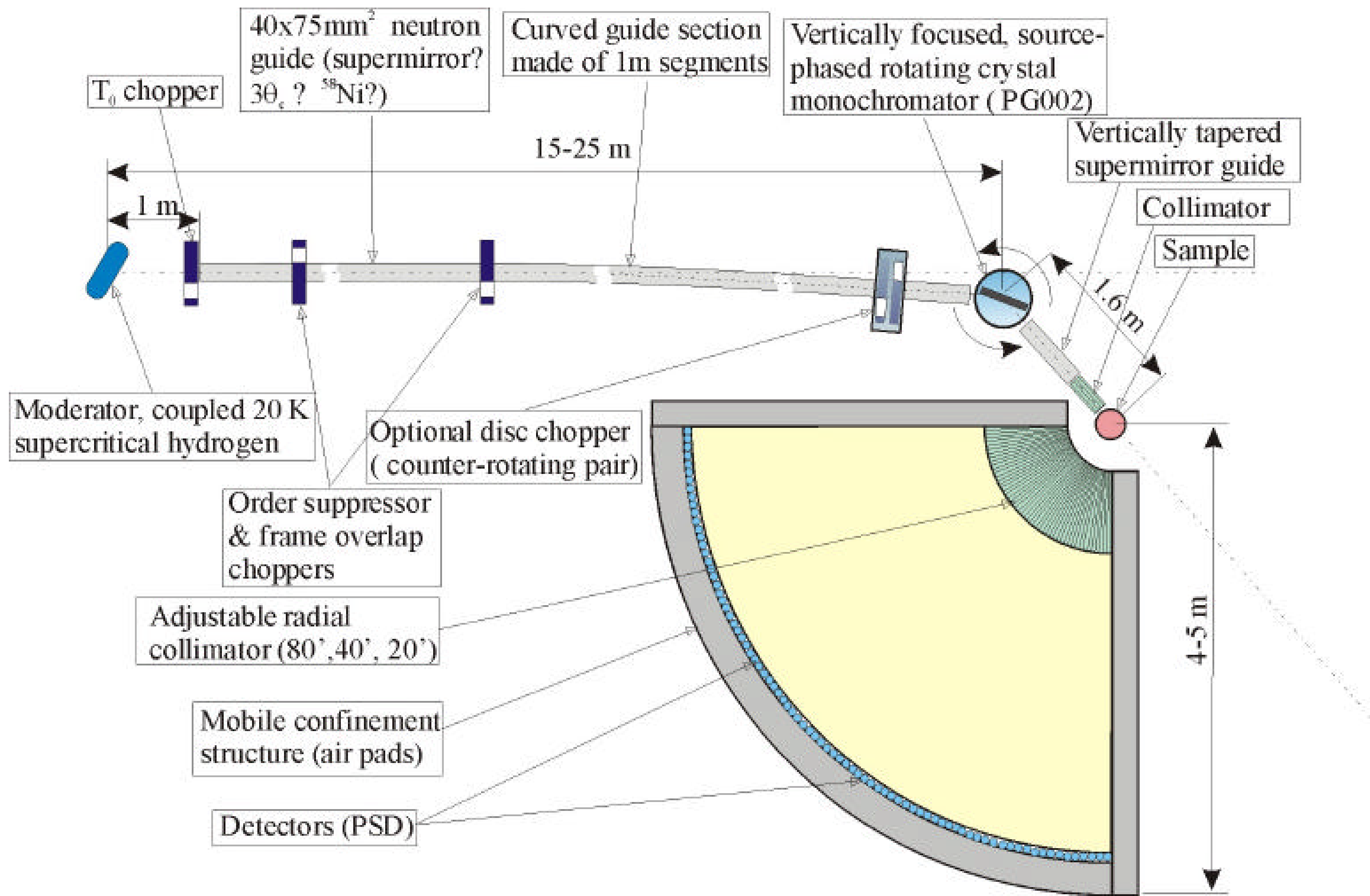
High resolution and low energy transfer

10-100 μeV Multichopper Spectrometer

- E = 2 - 20 meV
- Q = 0.1 - 4 Å^{-1}

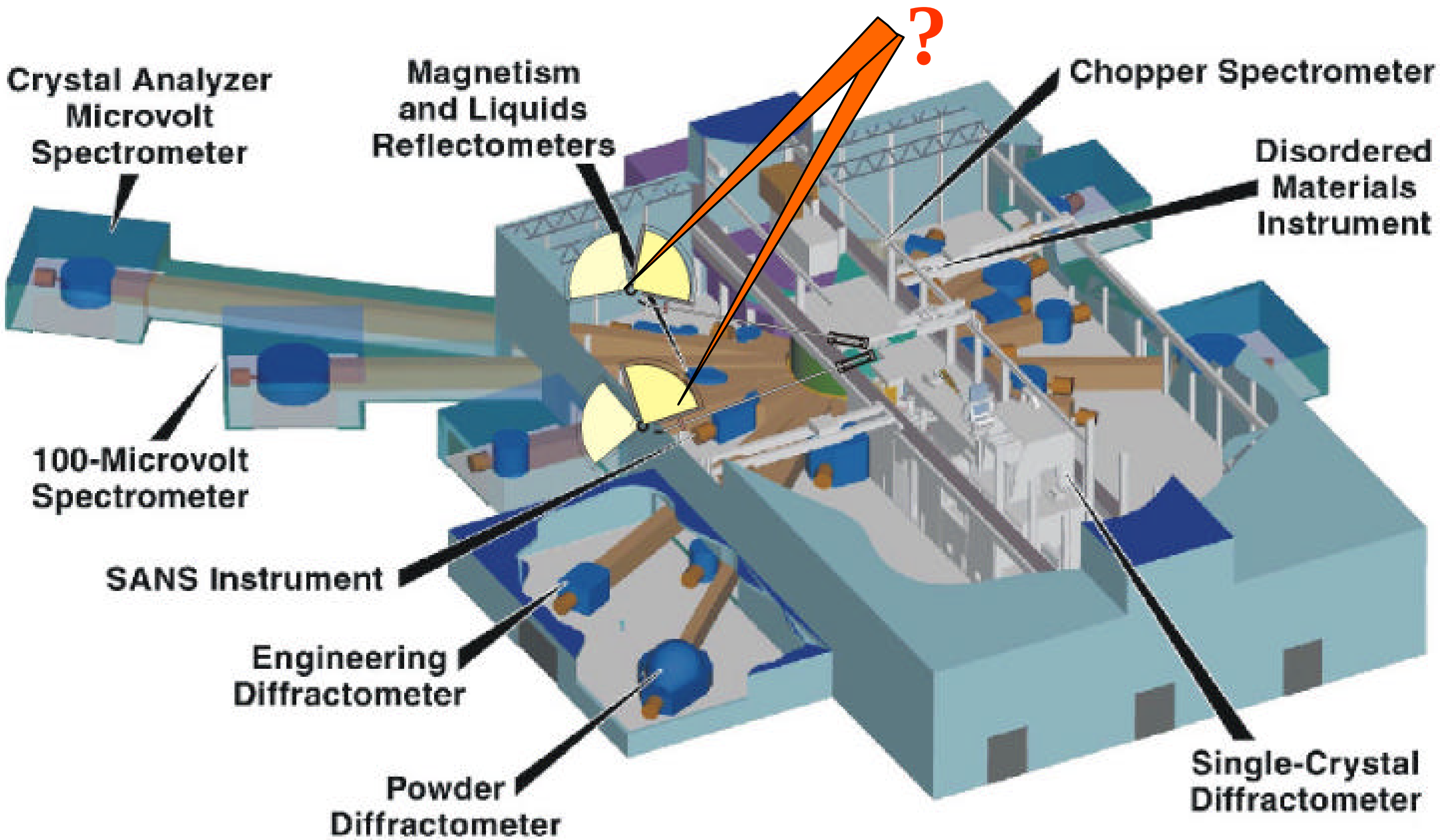


Schematic layout of the proposed Rotating Crystal Time-of-Flight Spectrometer



How does the instrument we propose fit SNS floor layout?

Needs rather short, 15 to 25 m primary flight path, but large, ~7-8 m radius floor area for the moving analyser bank and the sample table.

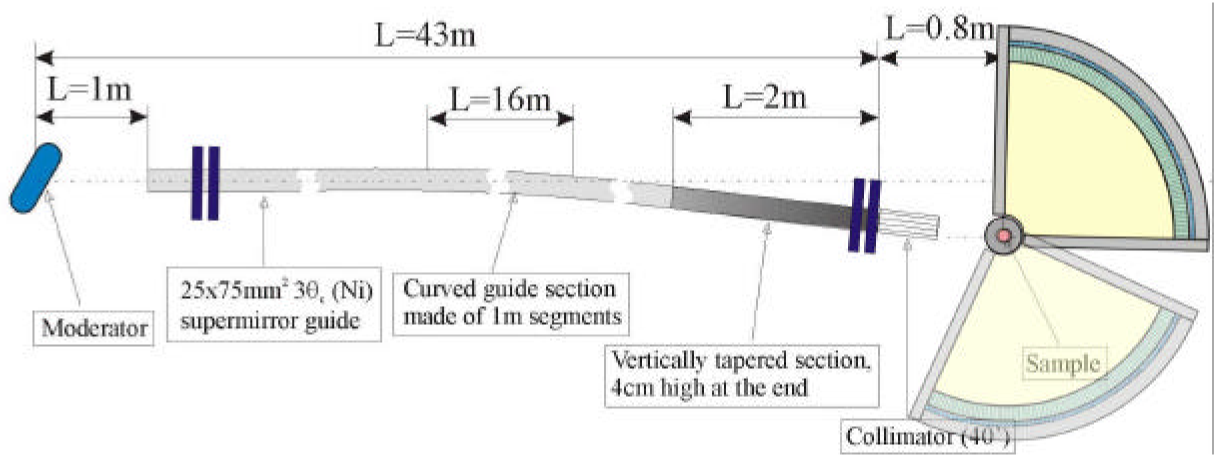


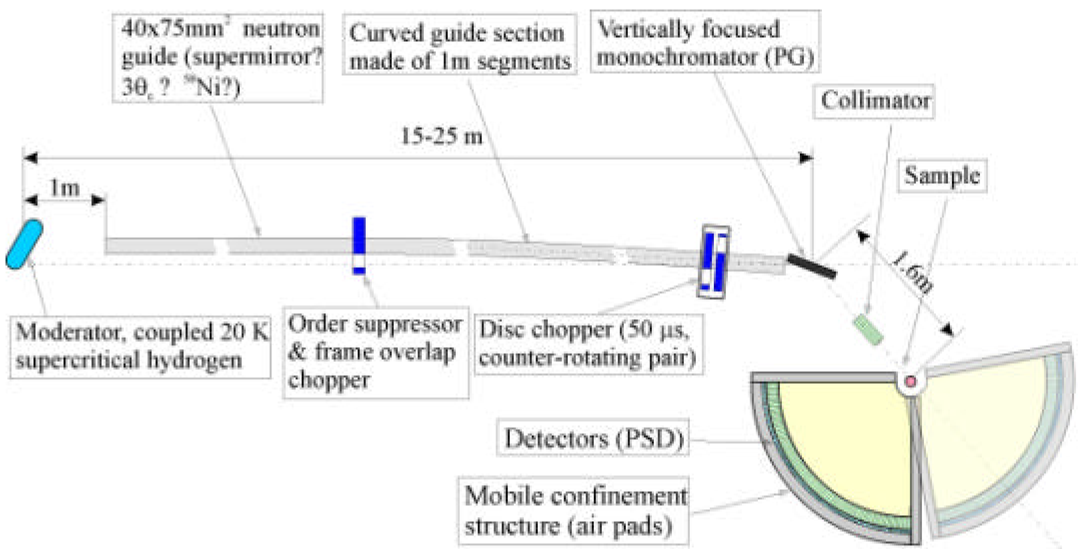
- Use the space following a shorter instrument?
- Occupy a “tangential” position with no other instruments on one side?

Evolution of our concept: from multi-chopper TOF to chopper-less hybrid spectrometer

We choose to optimize the instrument performance at E_i = 14.7 meV

Optimized layout of the direct geometry disc chopper spectrometer: curved guide loss ~6%, tapered section gain <1.4





Optimized layout of the direct geometry hybrid spectrometer with vertically focused crystal monochromator: expected gain from vertically focusing the beam >~ 2

Pro's and Con's of a Fermi Chopper

Advantages of a Fermi chopper

- short burst times can be achieved with wide beams
- works for very energetic neutrons
- beam height is not limited

Disadvantages of a Fermi chopper

- is a rotating collimator with curved slots: limits the beam horizontal divergence, does not take full advantage of the guide
- short burst times require tight collimation, i.e. reduced transmission and angular acceptance
- is optimized for a fixed set of incident energies, changing energy or resolution requires changing the rotor
- finite transmission away from the nominal angular position (especially at 180°) may lead to background and non-trivial beam contamination
- does not focus neutron beam on the sample

Pro's and Con's of a Disk Chopper

Advantages of a disc chopper

- rotation rate is not correlated with neutron energy, resolution can be semi-continuously varied
- energy can be changed without impacting on transmission

Disadvantages of a disc chopper

- small burst width cannot be achieved with wide beams because tensile strength limits maximum rotation rate
- transmission reduces when time for neutrons to traverse the disk becomes comparable with the slot open time (at lower neutron energies)
- order contamination may occur when multiple slot discs are used
- beam height is limited
- does not focus neutron beam on the sample

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 only to a reflected monochromatic beam: 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 beam energy is changed

What's Good About Rotating Crystal?

Defines the time structure of the neutron pulse at the sample: no chopper is necessary

Advantages of a rotating crystal monochromator

- short burst times can be achieved with wide beams without impacting on either transmission or collimation
- burst time decrease with decreasing neutron wavelength
- rotation rates are well below the tensile strength limit
- takes full advantage of the horizontal divergence introduced by the supermirror-coated guide
- no impact on vertical focusing
- possibility of time focusing (or defocusing) by changing the sense of rotation

Disadvantages of a rotating crystal monochromator

- introduces some Doppler broadening (but it decreases as the neutron wavelength increases)
- ?

Technical case for the rotating crystal monochromator

A PG(002) crystal array 23 cm wide is needed to reflect a 4 cm wide beam of 60 meV neutrons

- We assume a composite crystal monochromator, mounted on a 24 cm wide segmented vertically focusing device (GMI type), made of a high tensile strength Al alloy

- At a rotation rate of 240 Hz the peripheral velocity of the frame is 181 m/sec, well below the maximum peripheral velocity (500 m/s) for high tensile strength Al alloys

- At a rotation rate of 240 Hz the crystal velocity at the periphery of the spot illuminated by a 4 cm wide guide is about 5.1% of the velocity of a reflected neutron. For E_i > 14.7 meV this corresponds to a Doppler broadening of the incident energy distribution of less than 3.6%.

- Narrowing the beam reduces the Doppler broadening, a phased disc chopper upstream could be used for Doppler focusing

Performance of the rotating crystal monochromator

- PG(002) rotating crystal viewing the m=3 supermirror guide
- Crystal mosaic 1.2°, downstream angular acceptance α_1 = 0.66°
- Secondary flight path 4.0 m

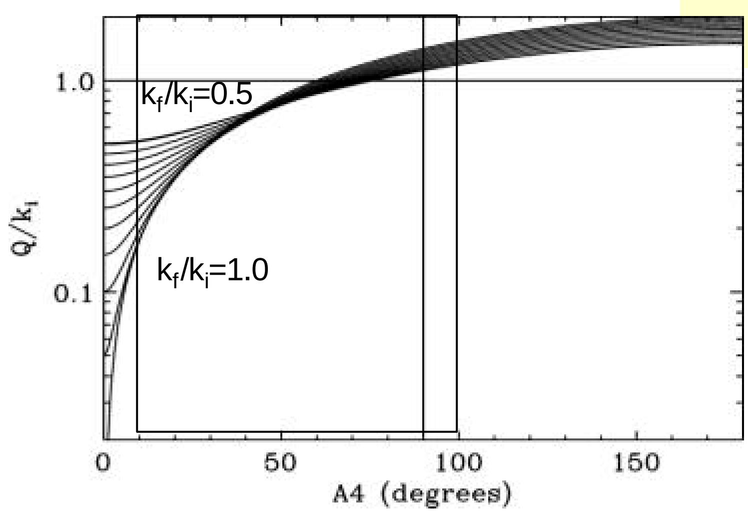
Crystal rotation rate (Hz)	Burst FWHM (μs)	Δt/t	ΔE/E
	Ei=5.0 meV (α_0 = 2.4°)		
240	32	0.0065	1.3%
180	42	0.0105	2.1%
120	63	0.0158	3.2%
60	126	0.0315	6.3%
	Ei=14.7 meV (α_0 = 1.4°)		
240	26	0.0111	2.2%
180	34	0.0146	3.0%
120	52	0.0223	4.4%
60	103	0.0441	8.8%
	Ei=60.0 meV (α_0 = 0.69°)		
240	22	0.0190	3.8%
180	29	0.0251	5.2%
120	43	0.0372	7.4%
60	87	0.0753	15.6%

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 5 m and for the t=40 µs burst width at the sample (FWHM)

	L_{SD}	$\Delta t/t$	$\Delta E/E$
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%



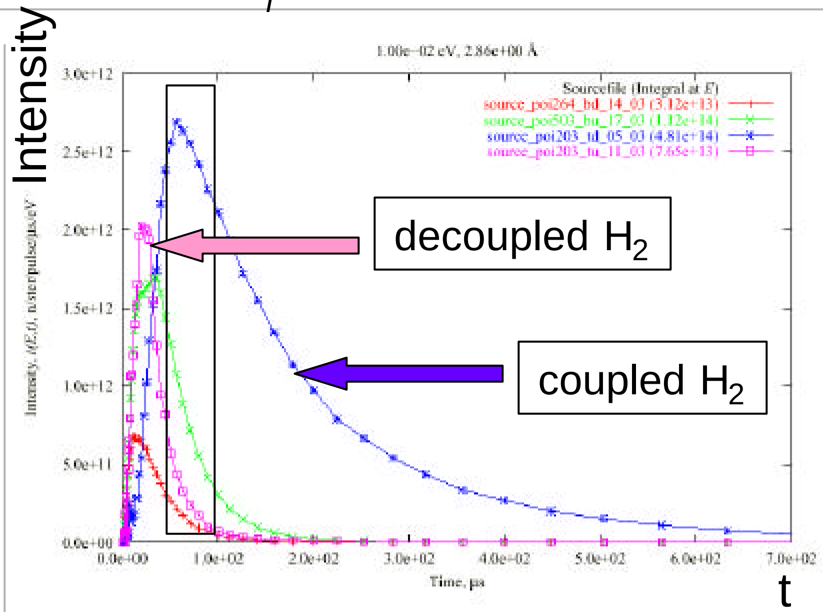
60° - 90° coverage of the scattering angle by the detector array gives simultaneous access to large enough interval in Q for $0.5<k_i/k_f<1$

Moving the analyzer is cost-effective!

Choice of the moderator

"Benchmark" the instrument performance at E_i = 15 meV

E_i = 10 meV



E_i = 20 meV

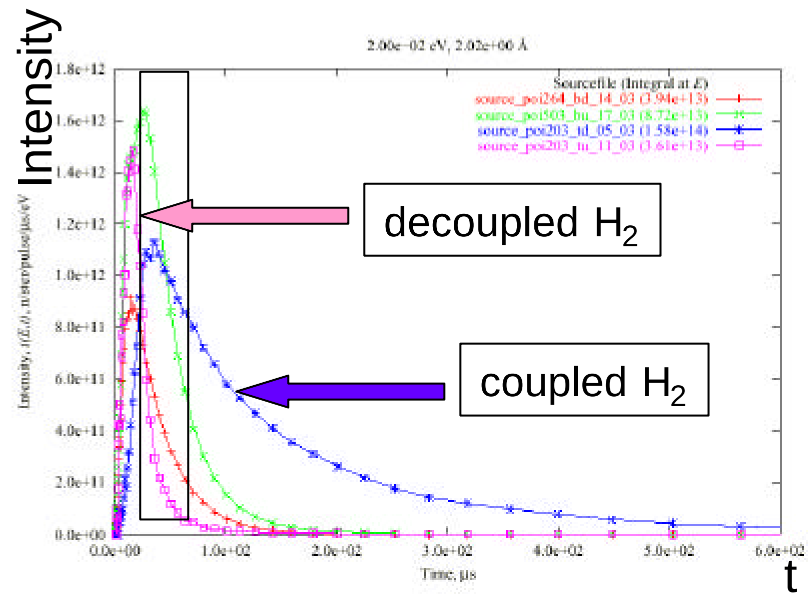
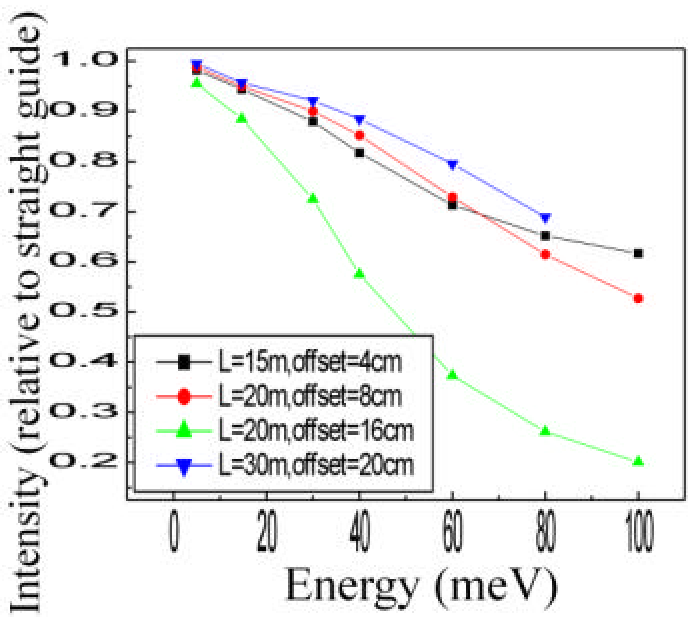


Figure of merit is the integral flux within 30-50 μs time window, defined by the length of the secondary flight-path

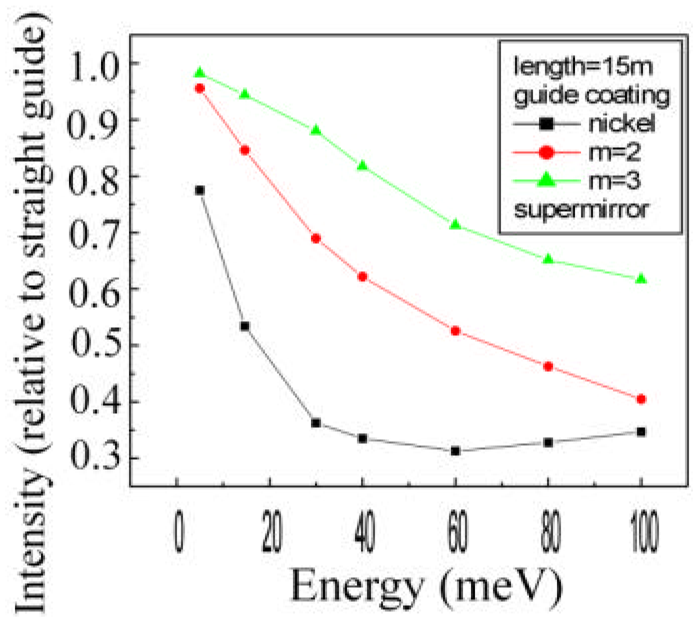
Coupled supercritical H_2 moderator

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

❑ Shorter (L = 15 m?) but narrower (3 cm?) guide may still be O.K.

Punchline: technical features of a proposed direct geometry hybrid instrument for the SNS

Efficient vertical focusing provides reasonable data collection rates even for very small samples !

- Spectrometer is optimized for
  - energy resolution dE/E~0.03-0.05
  - wavevector resolution dQ/Q~0.01-0.03
- High flexibility
  - continuous variation of the incident energy from 2.5 to 60 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
- Very low background
  - sample is 1.8 m away from the direct beam
  - scattering volume is well defined by collimators
- High sensitivity to small scattering cross-sections (signal to BG ratio)
- Can be operated at small scattering angles (near the forward direction)
- User friendly: allows for easy on-line data monitoring and analysis and experiment planning