HYSPEC - **Hybrid Spectrometer for the Single Crystal and Polarized Neutron Studies at the SNS**

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*Center for Neutron Scattering and Neutron Scattering Group*

Brookhaven National Laboratory

- Unique in its class
- Highest flux on small samples
- Easily adapted for polarized neutron studies
Outline

• Motivation (SMS)
• Science Case (SMS)
• IDT and Budget (SMS)
• Conceptual Design (IZ)
• Performance and Comparison (IZ)
• Summary (IZ)
Status

- Fall, 1999
  - BNL initiates an effort to design a spectrometer for the SNS
- December, 2000
  - Concept of the Hybrid Spectrometer formulated and adopted
- March, 2001
  - First presented to EFAC. Received positive reply
- Fall, 2001
  - Instrument Development Team formed
  - October: Workshop on the Hybrid Spectrometer held at BNL
  - Refined HYSPEC concept presented to EFAC
- January, 2002
  - HYSPEC IDT filed Letter of Intent with SNS
- April, 2002
  - Formal presentation to EFAC
- July, 2002
  - Letter of Intent accepted; Submit Scientific Proposal to EFAC
**Motivation**

SNS Inelastic Neutron Scattering Workshop\(^1\)
Argonne (11/99)

<table>
<thead>
<tr>
<th>Category</th>
<th>Instrument</th>
</tr>
</thead>
<tbody>
<tr>
<td>A.1</td>
<td>indirect geometry spectrometer, (backscattering), resolution 2 μeV (elastic position)</td>
</tr>
<tr>
<td>A.2</td>
<td>Direct geometry spectrometer (chopper), resolution ΔE/E ~ 1% (elastic position), E~10 – 1000 meV, continuous angular coverage</td>
</tr>
<tr>
<td>A.3</td>
<td>Spectrometer with 10 – 100 μeV resolution</td>
</tr>
<tr>
<td>B.1</td>
<td>Chopper, ΔE/E ~ 5% (elastic position), large angular coverage</td>
</tr>
<tr>
<td>B.2</td>
<td>Inverse geometry spectrometer, time focussed, ΔE/E ~ 1%</td>
</tr>
<tr>
<td>B.3</td>
<td>Triple axis-like instrument with high signal to noise</td>
</tr>
<tr>
<td>B.4</td>
<td>High Q chopper spectrometer with small ΔE/E</td>
</tr>
<tr>
<td>C.1</td>
<td>Spin echo spectrometer ΔE ~ 1 neV to 2 μeV</td>
</tr>
<tr>
<td>C.2</td>
<td>Brillouin scattering spectrometer, small Q, intermediate E</td>
</tr>
<tr>
<td>C.3</td>
<td>PRISMA-like spectrometer</td>
</tr>
</tbody>
</table>

- A and B category top priority - “potential day-one instrument”

Motivation from Workshop

- Small single crystal samples
  - Focussing Bragg optics
- Broad range of standard sample environments
  - Use of collimators and beam definers
  - Sample environment separate from detector vacuum
- Low background
  - Time of flight
  - Sample area out of direct beam
  - Use of collimators
- Vector $\mathbf{Q}$ in single crystals
  - Moveable detector and rotatable sample
- Polarization Analysis
  - Proven and maintenance-free technology
Motivation from Workshop

● Page 5 of Report:
“This [high time averaged flux] opens up the possibility of utilizing triple-axis like methods to examine details of excitations when the important physics can be found at specific, well defined regions of \(Q\) and \(E\) space”

● Recommended: “potential day-one instrument”
Science Case

- Quantum critical points
- Low-D magnetism
- Nanomagnetism and complex systems
- Disordered and weakly ordered phases
- Anomalous phonon behavior
- Strongly correlated electron systems
  - Hi $T_c$: YBCO experiment performed at ILL - IN22
Polarized Neutron Study on Resonant Mode in YBCO$_{6.85}$ (L.P. Regnault et al.)

IN22
Spin Flip
P // Q

- Much faster data collection
- Open new areas for polarized beam use

Rise due to increased counting time

Unpolarized

Sharp IC

Broad C
IDT Membership

I. Zaliznyak, co-PI BNL
S. M. Shapiro, co-PI BNL
G. Shirane BNL
J. Tranquada BNL
L. Passell BNL
D. Abernathy SNS
L. Daemen Los Alamos
M. Greven Stanford
B. Gaulin McMaster
K. Hirota ISSP
V. Kiryukhin Rutgers
G. Lander EITU
Y. Lee MIT
C. Majkrzak NIST
S. Nagler ORNL
R. Osborn ANL
L. P. Regnault CEN-Grenoble
J. Rhyne U. Missouri
C. Stassis Ames/Iowa St.
A. Zheludev ORNL

HYPSEC INSTRUMENT
DESIGN WORKING GROUP
I. Zaliznyak (BNL)
S. Shapiro (BNL)
L. Passell (BNL)
V. Ghosh (BNL)
(Monte Carlo Simulations)
S. Doran (SNS/ANL)
(Engineering Design)
## HYSPEC Budget Estimate

<table>
<thead>
<tr>
<th>Budget Category</th>
<th>Item</th>
<th>Cost</th>
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<tbody>
<tr>
<td><strong>Primary Flight Path</strong></td>
<td>Choppers</td>
<td>1400</td>
</tr>
<tr>
<td></td>
<td>Incident beam shielding</td>
<td>2300</td>
</tr>
<tr>
<td></td>
<td>Supermirror guides</td>
<td>500</td>
</tr>
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<td></td>
<td>Beam monitors</td>
<td>100</td>
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<tr>
<td></td>
<td><strong>SUB</strong></td>
<td>4300</td>
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<tr>
<td><strong>Monochromator</strong></td>
<td>Shielding</td>
<td>1000</td>
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<tr>
<td></td>
<td>Crystals and holder</td>
<td>400</td>
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<tr>
<td></td>
<td>Collimators</td>
<td>50</td>
</tr>
<tr>
<td></td>
<td><strong>SUB</strong></td>
<td>1450</td>
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<tr>
<td><strong>Sample Stage</strong></td>
<td>Goniometer, sample table</td>
<td>160</td>
</tr>
<tr>
<td></td>
<td>Ancillary equipment</td>
<td>250</td>
</tr>
<tr>
<td></td>
<td><strong>SUB</strong></td>
<td>410</td>
</tr>
<tr>
<td><strong>Analyzer, detector</strong></td>
<td>Collimator sets</td>
<td>200</td>
</tr>
<tr>
<td></td>
<td>Polarization benders</td>
<td>1000</td>
</tr>
<tr>
<td></td>
<td>PSD, electronics mounts</td>
<td>900</td>
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<td></td>
<td>Beam Controls-DAQ</td>
<td>140</td>
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<tr>
<td></td>
<td>Detector vessel</td>
<td>1500</td>
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<tr>
<td></td>
<td>Beam stop/get lost pipe</td>
<td>200</td>
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<tr>
<td></td>
<td><strong>SUB</strong></td>
<td>3740</td>
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<tr>
<td><strong>CAPITAL TOTAL</strong></td>
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<td>9900</td>
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<tr>
<td><strong>LABOR (1/3 Capital)</strong></td>
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<td>3300</td>
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<tr>
<td><strong>TOTAL</strong></td>
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<td>13200</td>
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</table>

**Budget estimates from:**

- SNS engineering group (11/01)
- HRCS Summary (7/02)

**Time Estimate:**

- 5 years from funding
HYSPEC: A Proposed Crystal-Time-of Flight Hybrid Spectrometer for the Spallation Neutron Source

Part 2: Conceptual design

- T₀ Chopper
- Disc Chopper
- Monochromator
- Goniometer
- Radial Collimator, or Bender Polarizers
- Flight Chamber (evacuated or Ar/He filled)
- Detectors
Why Hybrid Spectrometer?

- **Science challenges**
  - small samples
  - subtle features
  - polarization analysis
  - small signals, background-limited measurements

- **Need intensity boost**

- **Monochromator vertical focusing gain on SPINS@NIST**: factor ~3 even for m = 19 g sample (below)

![Graph showing intensity boost](image)
HYSPEC design choices: moderator

Time-spectra of the neutron intensity from different moderators for $E_i = 15.8$ meV

![Graph showing neutron intensity against time for different moderators.]

- 20K H$_2$ (coupled)
- 20K H$_2$ (decoupled)
- Ambient H$_2$O

Figure of merit is the total flux within $\Delta t = 40-80$ µs time window accepted by the spectrometer.

Moderators useful neutron flux

- Coupled 20K H$_2$
- Ambient H$_2$O

Neutron current through 4x12cm$^2$ guide entrance at 1.5 m from the moderator within $\Delta E = 2\%$ of $E_i$:
- 20 K coupled H$_2$ (MCSTAS interpolation)
- 20 K coupled H$_2$ (MCSTAS interpolation)
- H$_2$O (MCSTAS interpolation)
- MC calculation by E. Iverson

- Coupled supercritical H$_2$ moderator wins in thermal neutron range $E_i < 45$ meV
HYSPEC design choices: energy resolution

- For given incident pulse length \( \Delta t \) instrument energy resolution is determined by the analyzer flight-path.

- Sample and detector size contribution to the instrument resolution is less than 0.5% each.

- TOF analyzer energy resolution for the length of the secondary flight-path \( L_{SD}=4.5 \text{ m} \) and pulse lengths 40 \( \mu \text{s} \) to 80 \( \mu \text{s} \) is in the range 1.7% to 15%.

<table>
<thead>
<tr>
<th>( E_f )</th>
<th>( \Delta t/t_f )</th>
<th>( \Delta E/E_f )</th>
</tr>
</thead>
<tbody>
<tr>
<td>5.0 meV</td>
<td>0.0087 1.74%</td>
<td>40 ( \mu \text{s} )</td>
</tr>
<tr>
<td></td>
<td>0.0173 3.47%</td>
<td>80 ( \mu \text{s} )</td>
</tr>
<tr>
<td>15.0 meV</td>
<td>0.015 3.0%</td>
<td>40 ( \mu \text{s} )</td>
</tr>
<tr>
<td></td>
<td>0.03 6.0%</td>
<td>80 ( \mu \text{s} )</td>
</tr>
<tr>
<td>30.0 meV</td>
<td>0.021 4.25%</td>
<td>40 ( \mu \text{s} )</td>
</tr>
<tr>
<td></td>
<td>0.0425 8.5%</td>
<td>80 ( \mu \text{s} )</td>
</tr>
<tr>
<td>60.0 meV</td>
<td>0.03 6.0%</td>
<td>40 ( \mu \text{s} )</td>
</tr>
<tr>
<td></td>
<td>0.06 12.0%</td>
<td>80 ( \mu \text{s} )</td>
</tr>
<tr>
<td>90.0 meV</td>
<td>0.0368 7.36%</td>
<td>40 ( \mu \text{s} )</td>
</tr>
<tr>
<td></td>
<td>0.0736 14.7%</td>
<td>80 ( \mu \text{s} )</td>
</tr>
</tbody>
</table>
HYSPEC design choices: guide curvature

Flux on sample for different guide curvatures, parametrized by the corresponding offset at monochromator position.

- Straight guide with $m=3$ supermirror coating is an optimal solution.
HYSPEC performance: vertical focusing gain

Crystal-monochromator hybrid spectrometer (HYSPEC, top scheme) vs traditional “straight-through” TOF setup (MCST, bottom scheme).

- HYSPEC wins except at 5 meV, where both concepts are roughly equal.
HYSPEC performance: comparison with other inelastic instruments planned for the SNS

- MC simulations by MCSTAS, V. Ghosh (2002)
- CNCS, ARCS and HRCS intensities are re-scaled to HYSPEC energy resolution (such rescaling may over-estimate the actual intensity)

![Graph showing neutron flux on sample vs. energy (meV)]

- HYSPEC (no offset), coupled H₂
- CNCS¹, coupled H₂
- ARCS², H₂O
- HRCS², H₂O

¹CNCS model based on "Optimization...", J.V. Pearce et al.
²G. Granroth, Private communication
HYSPEC polarization analysis scheme: experimental demonstration

HYSPEC setup for polarization analysis

- Polarized incident beam is supplied by reflection from the vertically focusing Cu$_2$MnAl (Heusler alloy) crystal monochromator

10meV < $E_{i\text{pol}}$ < 90meV

- Polarization analysis of the scattered neutrons is done by a set of 11-22 supermirror-bender transmission polarizers, each 2 cm wide, 5 cm thick and 15 cm high,

5meV < $E_{f\text{pol}}$ < 25meV
HYSPEC layout in the polarized beam mode
HYSPEC performance in the polarized beam mode

Neutron energy 15meV

Bender width = 2cm
- All neutrons
- Spin up neutrons
- Spin down neutrons

Detector X co-ordinate (cm)
HYSPEC performance in the polarized beam mode

![Graph showing beam polarization vs. energy (meV) for straight and deflected beams.]

- **Straight beam**
- **Deflected beam**

![Graphs showing intensity vs. distance (mm) for different detector settings.]

- **ba45**
- **ba46**

[Brookhaven National Laboratory logo]
HYSPEC place in the SNS inelastic instrument suite

<table>
<thead>
<tr>
<th></th>
<th>HYSPEC</th>
<th>CNCS</th>
<th>ARCS</th>
<th>HRCS</th>
</tr>
</thead>
<tbody>
<tr>
<td>Incident energy range</td>
<td>5 – 90 meV</td>
<td>2 – 20(50?) meV</td>
<td>10 – 1000 meV</td>
<td>15 – 1000 meV</td>
</tr>
<tr>
<td>Maximum flux on sample</td>
<td>1.1 x 10⁷ at 15 meV</td>
<td>5.6 x 10⁶ at 5 meV</td>
<td>7.8 x 10⁶ at 100 meV</td>
<td>9.6 x 10⁶ at 100 meV</td>
</tr>
<tr>
<td>Energy resolution ΔE/E</td>
<td>0.017 – 0.15</td>
<td>0.01 – 0.1</td>
<td>0.02 – 0.05</td>
<td>0.015 – 0.05</td>
</tr>
<tr>
<td>Polarized beam</td>
<td>Yes</td>
<td>No</td>
<td>No</td>
<td>No</td>
</tr>
<tr>
<td>Intended sample size</td>
<td>4 (w) x2 (h) cm²</td>
<td>1.5 (w) x5 (h) cm²</td>
<td>5 (w) x7.5 (h) cm²</td>
<td>5 (w) x7.5 (h) cm²</td>
</tr>
<tr>
<td>Moderator-sample dist.</td>
<td>21.8m</td>
<td>36.2m</td>
<td>13.6m</td>
<td>17.5m</td>
</tr>
<tr>
<td>Sample-detector dist.</td>
<td>4.5 m</td>
<td>3.5 m</td>
<td>2.5 m</td>
<td>6.0 m</td>
</tr>
<tr>
<td>Angular acceptance</td>
<td>0.27 – 0.41 sR</td>
<td>3.1 sR</td>
<td>1.2 sR</td>
<td></td>
</tr>
<tr>
<td>Beamline #</td>
<td>15</td>
<td>5</td>
<td>18</td>
<td>17</td>
</tr>
<tr>
<td>Guide coating</td>
<td>m = 3</td>
<td>m = 3.5</td>
<td>m = 3 – 3.5</td>
<td>m = 3 – 3.5</td>
</tr>
<tr>
<td>Guide Apertures (width x height, cm²)</td>
<td>entrance 4x12.8\nmain 4 x 15\nexit 4 x 10</td>
<td>entrance 5 x 10\nmain 5 x 10\nexit 1.5 x 5</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Summary

- HYSPEC will be a unique resource for probing correlations in condensed matter for
  \[ E \in [5,90] \text{ meV} \quad \Delta E/E \in [0.05,0.15] \]
  \[ Q \in [0.3,10] \text{ Å}^{-1} \quad \Delta Q/Q \in [0.005,0.2] \]

- Worlds most intense thermal neutron beam at a pulsed source

- Can optimize range of energy transfer and resolutions for experiment

- Independent variation of Q and E resolution

- Polarization analysis capability

The ultimate question: Do we need HYSPEC?

Lead: Do we need 2 to 5 times larger flux on sample compared to other SNS spectrometers and a polarized beam option?

Our answer: Yes, we do.
Appendix. HYSPEC performance: monochromator resolution function

- Significant part of the incident beam intensity - in the unwanted high-E tail
- Requires a pulse-shaping chopper in a standard TOF setup
- Is removed by reflection from the monochromator in HYSPEC
Appendix. HYSPEC design choices: guide coating

Flux on sample for m=2, 3, and 3.5 supermirror guides (for 8 cm offset at the monochromator position).

□ Straight guide with m=3 supermirror coating is an optimal solution
Appendix. Intensity and pulse length of SNS moderators

![Graph showing intensity and pulse length of SNS moderators](image)