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HYSPEC: A Crystal Time-of-Flight Hybrid Spectrometer for the Spallation Neutron Source

S. M. Shapiro[1,2], I. Zaliznyak[2], L. Passell[1], V. Ghosh[1]

[1]*Center for Neutron Science, Brookhaven National Laboratory, PO Box5000, Upton, NY, USA*
[2]*Department of Physics, Brookhaven National Laboratory, PO Box5000, Upton, NY, USA*

Abstract

HYSPEC combines time-of-flight spectroscopy with focusing Bragg optics to enhance the flux on small single crystal samples. It will look at a coupled H_2 moderator and will use a 20-25 meter supermirror guide to transport the neutron beam. A counter-rotating chopper pair will monochromate the beam and determine the neutron burst width. A short distance from the chopper pair a vertical focusing crystal is placed in a drum shield that will focus the beam to a 2 cm height, thus maximizing the flux at the sample position. Collimators and beam definers will be placed before and after the sample, which will allow standard sample environment equipment to be used covering a wide range of temperatures and magnetic fields. About 200 He^3 position sensitive detectors will be housed in a moveable detector bank 4.5 m from the sample to cover a horizontal range of 60° and a vertical range of ±7.5°. HYSPEC can easily be converted to a polarized beam instrument by using a Heusler crystal for a monochromator, and supermirror benders for polarization analysis of the scattered beam. HYSPEC is a moderate resolution instrument optimized for an incident energy range of $5<E_I<60$ meV where it outperforms, in terms of flux on sample, the other inelastic instruments by at least a factor of 2 and up to a factor of 10.

1. Introduction

The study of phase transitions and novel ordered phases in complex systems remains at the forefront of condensed matter research. In studies of superconductivity, magnetism, ferroelectricity, colossal magnetoresistance, charge order, and other phenomena ofinterest to modern physics and technology one is interested in determining how each type of order occurs, including how and why it develops from the disordered state. This frequently requires parametric inelastic and elastic neutron scattering experiments over a narrow region of momentum and energy space on small specially grown single crystals. Up to now, most of these studies have been performed on triple axis spectrometers situated at steady-state neutron sources. Instruments at ISIS such as MAPS have made impressive strides in studies of single crystals, especially lower dimensional systems. However, as with all neutron instruments, experiments are still intensity limited. With the construction of the Spallation Neutron Source (SNS) at Oak Ridge National Laboratory, the available neutron flux will be more than an order of magnitude larger than that delivered at ISIS. This will definitely open up new areas of research and allow for novel instruments to be developed.

The Hybrid Spectrometer (HYSPEC) concept [1] combines time-of-flight spectroscopy with Bragg focusing optics used in triple axis spectrometers to enhance the flux of the pulsed beam that will be available at the SNS. HYSPEC fills a niche of dramatic importance to exciting areas of condensed-matter physics that is not filled by any other SNS inelastic instruments that have been considered to date. It is important to note that an SNS Inelastic Neutron Scattering Workshop held on 11/1/99 recommended that a spectrometer with almost identical charatersitics to HYSPEC be viewed as a "potential day-one instrument" [2]

2. The HYSPEC Spectrometer.

The objective in designing HYSPEC was to deliver the highest possible monochromatic flux to small (~cm-size) single crystals over a broad range of thermal and sub-thermal neutron energies (5-90 meV). Additional design considerations were (i) minimize beam related background such as that arising from sample environments,(ii) provide reasonably good and easily adjustable energy and momentum resolution, (iii) be readily adapted to polarization analysis, and (iv) permit rapid alignment of samples and easy installation of a broad variety of specialized sample environments. These criteria led to the direct geometry, hybrid concept shown in Fig. 1 with characteristics given in Table I.

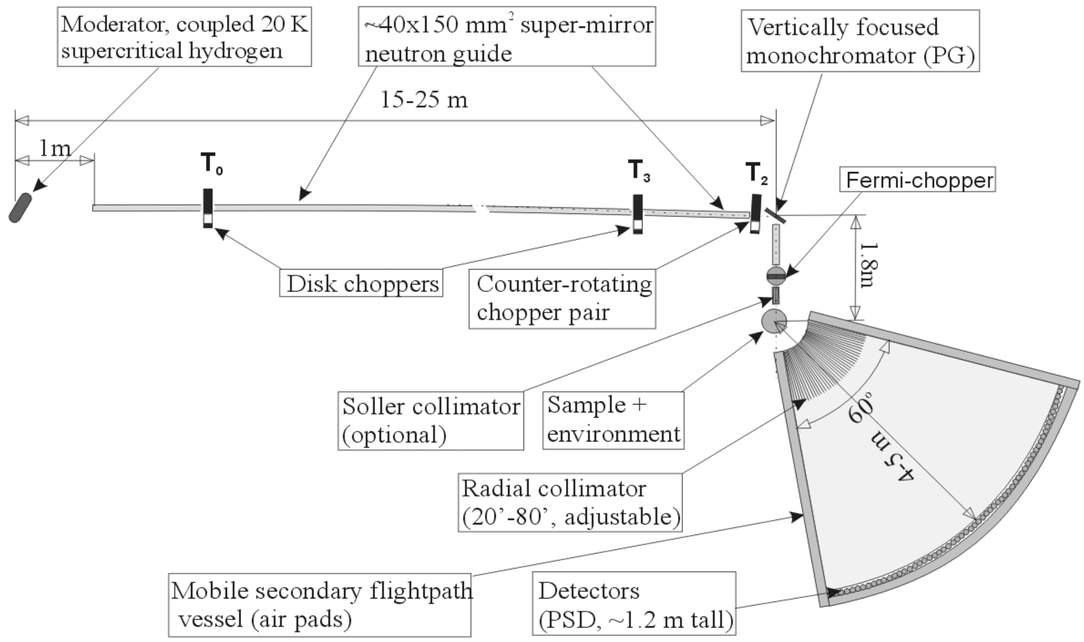


Figure 1: Schematic showing HYSPEC's principle elements.

2.1 Moderator Choice

Monte Carlo simulations have shown that to perform optimally over the incident neutron energy range of interest (5-90 meV), HYSPEC needs to be located on a beamline served by a coupled, 20 K, supercritical H_2 moderator. Because optimum performance requires that the monochromator and analyzer energy resolutions be reasonably well matched, the length of the monochromating section should not be much greater than 20 meters. It is also important that it ends at a place on the SNS experimental floor where there is sufficient space to accommodate both the rotating drum shield and the relatively extended time-of-flight analyzer and its associated shielding. The tentative position satisfying the above conditions, which has been assigned to HYSPEC is beam line 14B. The layout is shown in Fig. 2

Table I Instrument Parameters of HYSPEC

Moderator	Coupled, 20K, supercritical H_2
Incident energy	5 - 90 meV
Energy resolution	0.02 <ΔE/E <0.15 (for elastic scattering) depending on neutron energy and rotation rates of choppers
Q resolution	ΔQ/Q ~ 0.005 - 0.1
Primary flight path	Guide with expander and compressor sections 20-25 m long
Secondary flight path	4.5 m
Energy defining choppers	Counter-rotating disk and Fermi choppers. Maximum rotation rate 300Hz
Frame-overlap/order suppressor choppers	Disk choppers. Maximum rotation rate 60 Hz
Flux focusing crystal	Segmented, vertically curved PG and fluorinated mica. Heusler for polarized beam
Sample position	1.8 m from crystal
Beam size at sample (optimally focused)	4 (w) x 2 (h) cm^2
Detectors	188 2.5cm diameter position sensitive ^3He tubes. Horizontal pixel resolution 20 min. Vertical pixel resolution 20 min. Horizontal array acceptance: 60°. Vertical array acceptance: ±7.5°
Sample environment	Will accept all standard sample environment equipment

2.2 Neutron guides and choppers

The primary spectrometer consists of a 20-25 meter long straight guide with a center section composed of 40 mm wide by 150 mm high, supermirror-coated modules and with 40 mm wide expander sections at each end. A T_0 chopper is placed about 6m from the moderator to block the gamma rays and high energy neutrons emitted in the earliest part of the source pulse. The frame overlap chopper (T_3) assures that unwanted, higher-order neutrons are removed. Also, its rotation rate can be reduced when necessary to block alternate source pulses in cases where the scattered energy spectrum is so broad that spectral overlap becomes a problem. In most cases, the neutron wavelength selection will be done by counter rotating disk choppers (T_2) which will, along with the monochromator crystal, define the energy of the beam and the spectral and time width of the pulse at the sample position, the latter being the main factor in determining the energy resolution of the time-of-flight analyzing section. In those cases where higher energy resolution is needed the time width of the sample pulse could be further reduced by the addition of a Fermi chopper (T_4). This chopper would have short, straight, slots and a vertical axis of rotation and be located in the shield immediately upstream of the collimator. Like the counter–rotating disk choppers, it would rotate at integral multiples of the source frequency, with the highest rotation rate of ~500 sec^{-1}

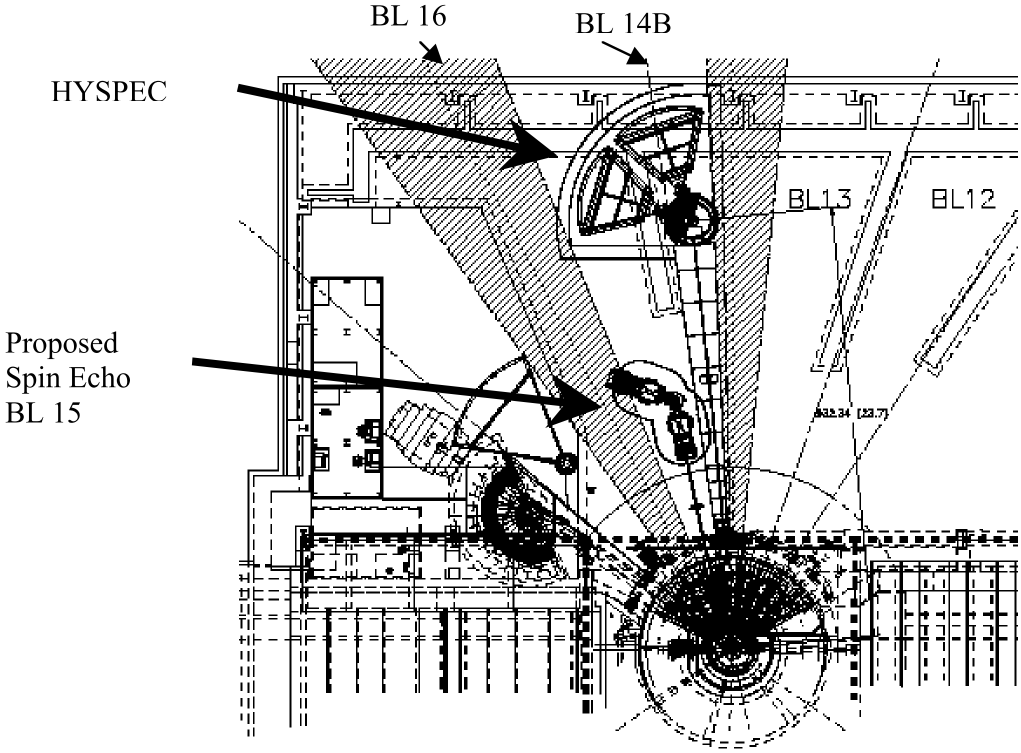


Figure 2: Proposed location of HYSPEC on Beam Line BL 14B on SNS experimental floor

2.3 Focusing crystal and rotating drum

The unique feature of HYSPEC is the use of a vertically focusing crystal located in a well shielded drum to reduce the beam height to about 2 cm. Monte Carlo methods have shown that use of a crystal to focus the beam is more efficient than using tapered focusing guides. For incident energies >5.0meV individual pyrolytic graphite (PG) plates will be attached to a segmented holder that will allow the radius of curvature to be varied. For optimum performance an anisotropic mosaic with a broad horizontal mosaic (~1.0°) and narrow vertical mosaic (0.3) is desirable. To this end, three ZYA grade PG plates stacked with spacers to slightly offset the angles between them will be used to increase the horizontal mosaic. This so-called “fan arrangement” has been demonstrated to expand the horizontal mosaic but leave the vertical mosaic (and thus the vertical focusing properties of the crystal) unchanged. At incident energies below 5 meV the monochromator scattering angles become very large and an equivalent crystal composed of fanned plates of fluorinated synthetic mica or intercalated graphite will be used.

A drum-like shield, similar to those at reactors, will be used to house the focusing crystal and provide the necessary shielding to reduce radiation and background near the sample area. At the beam exit there is provision for collimators which can control the q-resolution as well to reduce background from sample environments.

2.4 Sample area

Another important unique attribute of HYSPEC is that it can accommodate specialized sample environments. This is due to the location of collimators upstream and downstream of the sample which restrict the horizontal field of view of the detectors to the sample area alone. The HYSPEC sample axis will not have to be part of the instrument vacuum system as in other existing and planned inelastic instruments. Thus we expect to be able to employ conventional cryostats, magnets, furnaces, pressure cells, etc. without creating any significant, sample- environment-related background problems.

2.5 Analyzer/Detector

Scattered neutron energy analysis would be done by time-of-flight alone. We propose using a 4.5 meter radius array in a gas-tight tanke made up of 188 one-dimensional, position-sensitive, tube-type ^{3}He detectors 2.5 cm in diameter and 1.28 meters long, centered at the sample position. A set of radial collimators (with horizontal angular acceptances of 20, 40, 60 and 80 minutes) placed after the sample and would restrict the detector horizontal field of view to the sample area alone. Horizontal and vertical resolutions of an individual pixel are envisioned as being respectively 20 and 20 minutes of arc. Additionally, the array would span a 60 degree arc horizontally and have a vertical acceptance of ± 7.5 degrees with respect to the scattering plane. Currently, it is previewed to be mounted on air pads on a "tanzboden" so that it could both move with the drum shield and be rotated about the sample axis to permit accurate positioning with respect to the monochromatic beam incident on the sample. The tank area would most likely be gas filled and located in a fixed, well shielded housing.

3. Polarization Analysis

One of the particularly attractive features of HYSPEC is that it can be quickly and easily adapted to polarization analysis using well-established and maintenance free techniques. For selecting the incident neutron polarization it will be a simple matter to replace the PG crystal by a Heusler (Cu_2MnAl) crystal set for the (111) reflection. This reflection has the property that the nuclear and magnetic scattering lengths are equal so only one spin state is reflected. Studies [3] have shown that the polarization is in excess of 95% when the Mn moments are fully aligned. Also the (111) Bragg reflecting efficiencies can approach those expected for an ideally imperfect crystal such as PG.

One cannot use a Heusler crystal to analyze the polarization of the scattered beam and still take advantage of the extended angular acceptance of HYSPEC. We plan to use the broadband supermirror-benders transmission polarizers inserted into the collimator region of the detector bank. This type of analyzer is a short, curved multi-channel guide with magnetically aligned, polarization-selective Fe-Si supermirror films on the channel walls. Since, the neutrons of one spin state will follow the curvature of the guide, while the other spin state will go straight through the guide, they will be spatially separated [4] by 7 cm at the detector bank and both polarizations can be measured simultaneously. In order to make the most effective use of the extended angular acceptance an array of bender analyzers would need to be installed. Nineteen bender analyzers could be positioned within the solid angle subtended by the detector array. By use of two bender arrays optimized for 5.0 and 15 meV, respectively, it is possible to span the scattered neutron energy range from 3 to 18 meV.

4. Performance of HYSPEC and comparison with other SNS inelastic instruments.

Of the many special and unique features of HYSPEC, the most important is the utilization of the superior focusing properties of curved crystals to concentrate the monochromatic flux on sample. To quantify the gain, we performed a number of MCSTAS, Monte-Carlo based simulations to compare HYSPEC's flux on sample with that of the other proposed SNS inelastic instruments:

CNCS: Cold Neutron Chopper Spectrometer situated on a couple H2 moderator, BL 5

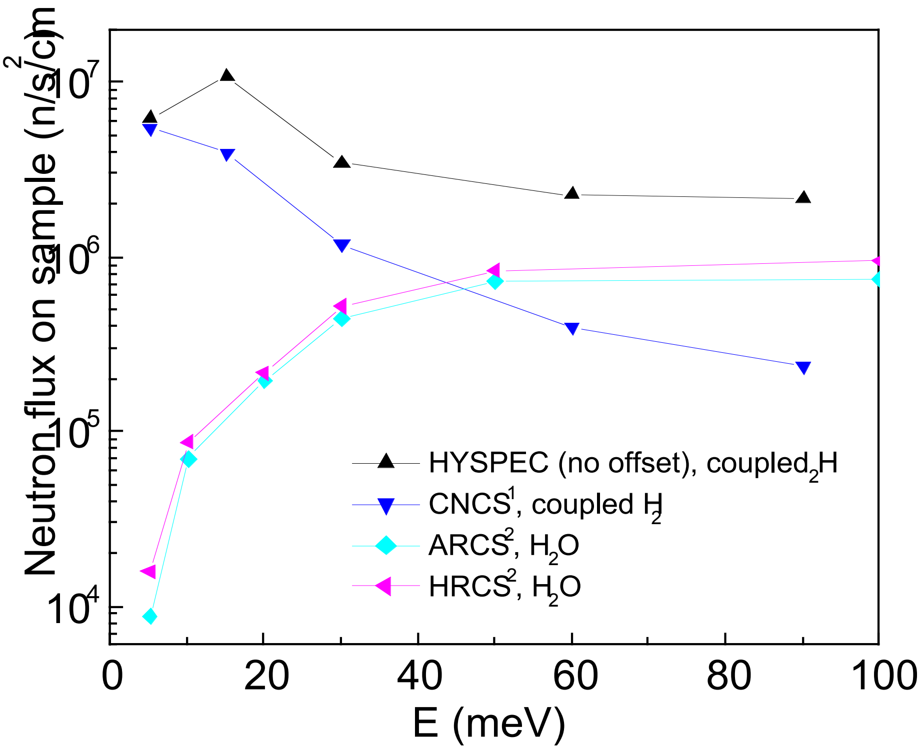
ARCS: Wide-angle chopper spectrometer looking at a water moderator on BL 18

SEQUOIA: High-resolution chopper spectrometer looking at the water moderator on BL 17.

Since these instruments are optimized for different energy ranges and resolutions care must be taken in making these comparisons. Fig. 1 shows the flux on sample as a function of incident energy for HYSPEC. The Monte Carlo calculations were for a chopper rotation frequency of 300 Hz, a constant slot width of 4 cm, and a sample size of 2 x 2 cm^2. The energy resolution, $\Delta\omega/\omega$, varies over the range of incident energies of 5 – 90 meV from about 2% to 10%, respectively. To compare with HYPSEC the flux estimate of other instruments was multiplied by the ratio of the energy resolution of HYPSEC to that of the other instruments. The results in Fig. 3 shows that HYSPEC has superior performance in the designed energy range of 5 - 90 meV. The low flux on ARCS and HRCS (now called SEQUOIA) for energies below 50 meV is due to their placement on a water moderator.

Ganroth and Abernathy [5] performed similar MCSTAS calculations to compare the performance of different instruments but used a different normalization approach. For each instrument (CNCS, ARCS, and SEQUOIA) they matched the energy resolution of HYSPEC by adjusting the chopper frequency and slot width. This results in unrealistic operating conditions for these instruments but it is another valid method for normalization. The results are similar to Fig. 3 in that HYSPEC gives a superior performance in the range of 5-50 meV, which bridges the cold and thermal to the epithermal regime of the other 3 instruments.

It should be noted that the higher flux on sample provided by HYSPEC is due to the more relaxed energy resolution and coarser vertical resolution than the other instruments. However, in pioneering studies of new materials this is not seen as a disadvantage and HYSPEC will open up new areas of application of pulsed neutron sources to studies of single crystals



[1]CNCS model based on "Optimization...",J.V.Pearce et al.

[2]G.Granroth, Private communication

Figure 3. Calculated flux on sample for HYSPEC and other inelastic spectrometers[1]

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