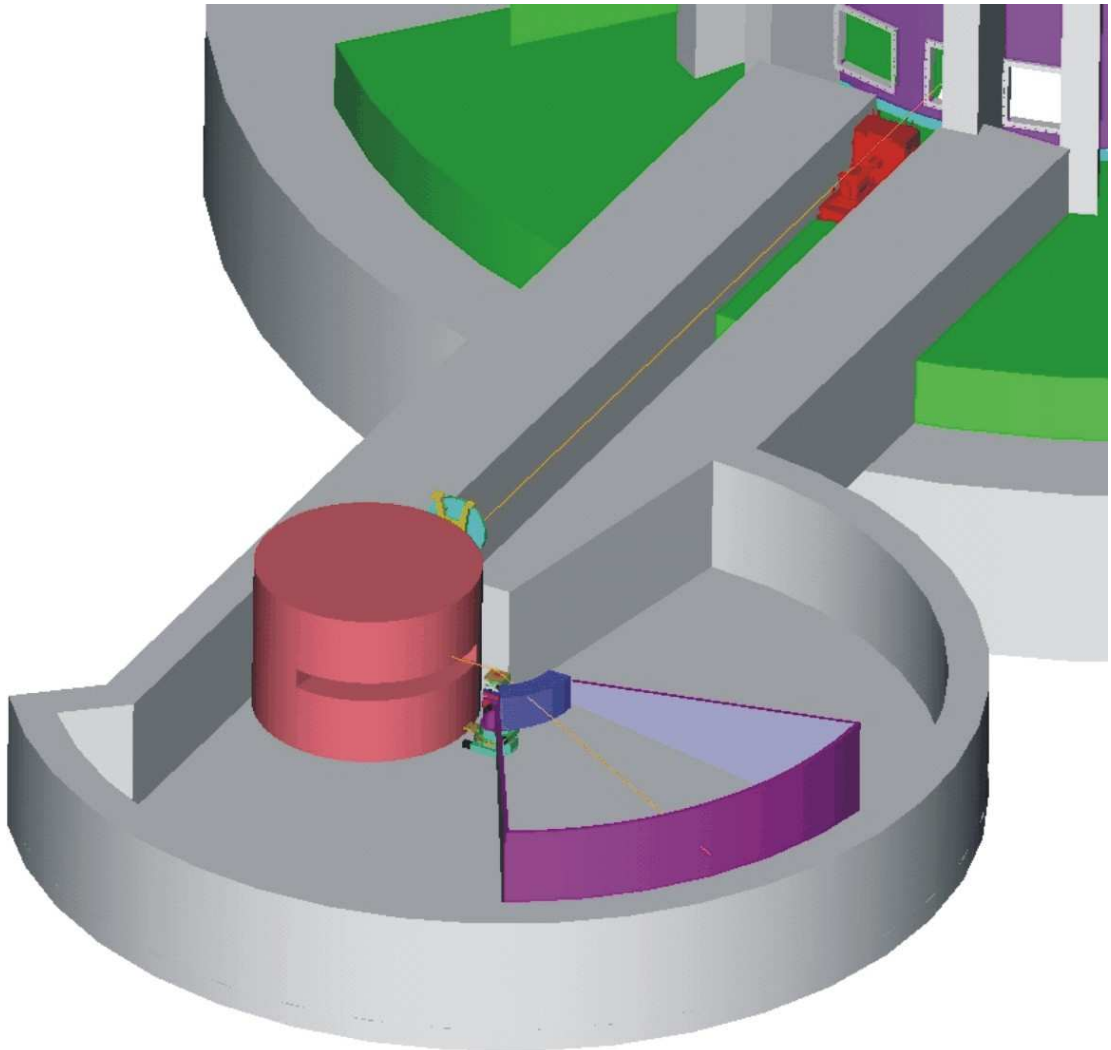


## **HYSPEC: A Crystal-Time-of-Flight Hybrid Spectrometer for the Spallation Neutron Source**



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## EXECUTIVE SUMMARY:

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, etc., one is interested in determining how each type of order occurs, including how and why it arises from the disordered state. The energy scale for excitations that have an impact on ordering is typically on the order of a few to tens of meV; this is the same energy scale for excitations that impact transport properties. The intensities and energy resolutions obtainable with thermal neutrons are ideal for such inelastic studies. At the same time, one needs to be able to detect and monitor the relevant order parameter through elastic diffraction measurements, which frequently involves measurements of superlattice peaks that may be extremely weak. Often one wishes to study correlations that have not achieved long-range order, in which case one must measure diffuse scattering and be able to discriminate elastic from inelastic contributions. In many cases understanding the order of interest requires studying how it is modified or induced by an extreme environment, such as a strong magnetic field, very low temperature, or high pressure; this is best accomplished by decoupling the sample environment from the detector system. In order to exploit the full power of neutron scattering to distinguish magnetic from nuclear scattering, it is necessary to implement polarization analysis, with polarization sensitivity in both the incident and scattered beams. Finally, in order to discover new phenomena, and to not simply characterize phenomena that have been discovered at other facilities, one has to be able to work with small crystals, thus requiring that a spectrometer focus as much flux as possible into a small spot size.

Up to now, the combination of requirements described above has been met only by triple-axis spectrometers at steady-state sources. Here we present the case that by combining time-of-flight spectroscopy with Bragg focusing optics and the enhanced flux of the pulsed beam that will be available at the SNS, one can build an instrument that not only satisfies our needs, but which will also significantly exceed the performance of the best triple-axis spectrometers at the best steady-state sources. The instrument that we propose, HYSPEC, fills a niche of dramatic importance to exciting areas of condensed-matter physics, one that is not competitively covered by any of the other SNS instruments that have been considered to date.

HYSPEC was approved by the SNS Experimental Facilities Advisory Committee (EFAC) at its October, 2002 meeting. Provisionally it has been assigned beam line which looks at a coupled, supercritical H<sub>2</sub> moderator (BL 15). To transport the beam from the moderator to the sample the instrument will have a straight, 20 to 25 meter long, m=3 supermirror guide that will incorporate T<sub>0</sub>, frame overlap and order suppressing choppers along its length and, near its downstream end, a counter rotating chopper pair that will serve to define the neutron burst width and incident energy. A short distance downstream of the counter-rotating chopper pair, the monochromatic beam will impinge on either a pyrolytic graphite or (for polarized beam studies) Heusler alloy vertical-focusing crystal mounted in a drum shield with adjustable exit angle. Because vertical focusing by crystals is extremely efficient, the 4(w) x 15 (h) cm<sup>2</sup> beam exiting the guide will be reduced to an area as small as 4(w) x 2(h) cm<sup>2</sup>, thus maximizing the flux at the sample position. A series of collimators and beam definers will be placed immediately upstream

of the sample and a set of radial collimators in the detector bank just downstream of the sample. In the polarization-analysis mode the radial collimator would be replaced by a set of 19 Fe-Si supermirror benders that would make it possible to measure simultaneously both spin-flip and non-spin-flip processes. Detection of the neutrons scattered by the sample will be done by 188 <sup>3</sup>He position-sensitive detectors housed in a moveable detector bank 4.5 m from the sample that will cover a horizontal angular range of 60° and a vertical range of 15°.

HYSPEC's flux-on-sample was compared to the other planned inelastic instruments CNCS, ARCS and HRCS (which have overlapping energy ranges and resolutions) using the MCSTAS Monte Carlo simulation program. For HYSPEC, the maximum flux on sample at a 3% energy resolution was found to be  $1.1 \times 10^7$  n/cm<sup>2</sup>/sec at 15 meV. This is a factor of two more than the maximum flux of CNCS, which is at an energy of 5 meV, and about ten times more than maximum flux of HRCS and ARCS, which occurs at an energy around 100 meV. This high sample flux combined with TOF analysis and the wide angular acceptance of the detector array means that a given scattered neutron spectrum will be collected in an order of magnitude less time than on existing single crystal sample instruments.

The easy adaptability of HYSPEC to polarization analysis is unique among the suite of SNS inelastic instruments. To produce a focused, polarized beam the PG crystal is simply replaced by a vertical focusing Heusler alloy crystal. Analysis of the polarization of the scattered neutrons will be done with a set of 19 broad-spectrum Fe-Si supermirror benders downstream of the sample: a well-established and extremely reliable technology. Because the sample-to-detector distance is large, the spin-flip and non-spin-flip parts of the scattering will fall on different groups of detectors. This will allow both to be measured simultaneously.

HYSPEC Instrument Development Team includes an international group of prominent scientists interested in single crystal inelastic neutron scattering. They provide input to the design of the spectrometer, high international visibility of the project, and will assure a high level of scientific productivity in the future. We are encouraged by the recent discussion with the French IDT member who has indicated that the Atomic Energy Commission (CEA) may participate in the HYSPEC project.

Finally, it should be noted that an SNS Inelastic Neutron Scattering Workshop held on 11/1/99 at ANL recommended that a spectrometer with almost identical characteristics to HYSPEC be viewed as a "potential "day-one" instrument" (Appendix B).

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

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## 1. INTRODUCTION

This document lays out a proposal by the Instrument Development Team (IDT) composed of scientists from leading Universities and National Laboratories to design and build a conceptually new high-flux inelastic neutron spectrometer at the pulsed Spallation Neutron Source (SNS) at Oak Ridge. This instrument is intended to supply users of the SNS and scientific community, of which the IDT is an integral part, with a platform for ground-breaking investigations of the low-energy atomic-scale dynamical properties of crystalline solids. It is also planned that the proposed instrument will be equipped with a polarization analysis capability, therefore becoming the first polarized beam inelastic spectrometer in the SNS instrument suite, and the first successful polarized beam inelastic instrument at a pulsed spallation source world wide.

The proposed instrument is designed primarily for inelastic and elastic neutron spectroscopy of single crystals. In fact, the most informative neutron scattering studies of the dynamical properties of solids nearly always require single crystal samples, and they are almost invariably flux-limited. In addition, in measurements with polarization analysis the available flux is reduced through selection of the particular neutron polarization, which puts even more stringent limits on the feasibility of a particular experiment. To date, these investigations have mostly been carried out on crystal spectrometers at high-flux reactors, which usually employ focusing Bragg optics to concentrate the neutron beam on a typically small sample. Construction at Oak Ridge of the high-luminosity spallation neutron source, which will provide intense pulsed neutron beams with time-averaged fluxes equal to those at medium-flux reactors, opens entirely new opportunities for single crystal neutron spectroscopy. Drawing upon experience acquired during decades of studies with both crystal and time-of-flight (TOF) spectrometers, the IDT has developed a conceptual design for a focused-beam, hybrid time-of-flight instrument with a crystal monochromator for the SNS called HYSPEC (an acronym for hybrid spectrometer). The proposed instrument has a potential to collect data more than an order of magnitude faster than existing steady-source spectrometers over a wide range of energy transfer ( $\hbar\omega$ ) and momentum transfer ( $Q$ ) space, and will transform the way that data in elastic and inelastic single-crystal spectroscopy are collected. HYSPEC is optimized to provide the highest neutron flux on sample in the thermal and epithermal neutron energy ranges at a good-to-moderate energy resolution. By providing a flux on sample several times higher than other inelastic instruments currently planned for the SNS, the proposed instrument will indeed allow unique ground-breaking measurements, and will ultimately make polarized beam studies at a pulsed spallation source a realistic possibility.

Even though the polarized beam option was not considered at the time, a spectrometer with performance characteristics similar to those of HYSPEC was identified as one of the potential “day-one” inelastic instruments for the SNS at the Inelastic Neutron Scattering Workshop<sup>1</sup> organized by the SNS at Argonne in 1999. It was included as such in the Workshop recommendations, along with six other instruments, four of which are

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<sup>1</sup> Report on the SNS Inelastic Neutron Scattering Workshop held on 11/1999 at ANL, SNS Document IS-1.1.8.2-8004-MM-A-00 (2000), Appendix B.

currently approved, with three of those having already been funded and now under construction. This proposal is a request by the IDT for funding for the engineering and construction of the HYSPEC spectrometer on a beamline served by a coupled, 20 K supercritical hydrogen. The proposal is organized as follows. In the next section we outline the general scientific motivation for the proposed instrument by presenting some of the research programs proposed for HYSPEC by the IDT members. Section 3 contains an overview of the instrument conceptual design, a discussion of the principles of polarized beam operation, a summary of the instrument performance characteristics and some future considerations. Section 4 outlines the structure of the HYSPEC Instrument Development Team, a management plan is discussed in Section 5, and a tentative budget estimate is given in Section 6 (and Appendix D). CVs of key IDT members are attached in Appendix A. For reference, an excerpt from the report of the SNS Inelastic Neutron Scattering Workshop held on 11/1/99 at ANL, SNS Document: IS-1.1.8.2-8004-MM-A-00, is attached in Appendix B. Finally, Appendix C is a draft of the HYSPEC Top Level Specifications which contain a detailed list of the instrument requirements to implement the conceptual design as proposed by the IDT.

## **2. SCIENTIFIC MOTIVATION: MEETING THE NEW CHALLENGES**

Much of our current understanding of atomic-scale structure and the dynamical properties of solids and liquids was gained by virtue of neutron scattering studies. Inelastic neutron spectroscopy provided physicists with an unprecedented, detailed access to phonon dispersions, magnetic excitation spectra, soft-modes and critical dynamics at phase transitions, unrivaled by other experimental techniques. Because the neutron only interacts very weakly with matter, it is essentially a non-perturbing probe of the matter's inner structure and dynamics, not sensitive to charges or surface layers. Therefore, unlike techniques where photons, or charged particles (eg electrons, muons), which significantly modify the local electronic environment, are used, neutron spectroscopy allows determination of the intrinsic, un-perturbed physical properties of materials. By the same virtue, the neutron is a highly penetrating and non-destructive probe, allowing the investigation of microscopic properties of bulk materials (and not just their surface layers), and studies of samples embedded in a complex sample environment, such as cryostats, magnets, pressure cells, etc. In fact, the ability to accept a variety of devices creating extreme sample environments was one of the key factors that determined tremendous success of the modern reactor-based neutron spectrometers. Finally, determination of how partial cross-sections depend on the neutron spin polarization through the use of various beam-polarizing devices gives an unrivaled opportunity to separate the structural and magnetic phenomena on the atomic scale. Incorporating and optimizing these unique features of the neutron scattering technique in the design of a neutron spectrometer is extremely important.

The discovery of new materials and novel unexpected phenomena along with the advent of new experimental techniques invariably leads to major advances in condensed matter science. One example is the discovery of strongly correlated electron systems, including heavy-fermions to high- $T_c$  superconductors to manganites exhibiting giant magneto-resistance effects. These materials present new types of macroscopic behavior with a strong potential for future technological applications, which require detailed understanding at the microscopic level. The neutron scattering studies which are

indispensable for such understanding represent a significant experimental challenge. First of all, new materials are usually only available in small quantities. Secondly, the scattering intensities associated with the interesting features in the electronic structure are often intrinsically small. Finally, because several contributions to the microscopic electronic Hamiltonian in these systems are of comparable importance for determining their macroscopic bulk properties, direct discrimination between the magnetic scattering by electronic spin and structural/vibrational scattering by the means of polarization analysis is vital.

The goal of the present IDT is to design and build an instrument which, using the unique, high-flux, pulsed neutron beam at the SNS, would meet the challenges posed for neutron spectroscopy by new scientific discoveries and breakthroughs in the synthesis of the new materials. There is a large number of problems that are currently at the forefront of condensed matter physics and demonstrate the need for an instrument with the unique capabilities of HYSPEC. In this section we present some examples which illustrate how HYSPEC is expected to significantly extend the reach of modern experimental condensed matter science.

## **2.1. Functional Materials**

Fundamental understanding of the microscopic processes governing physical phenomena in complex functional materials is key to technological progress. HYSPEC is an indispensable experimental tool that is needed to obtain such understanding.

### **2.1.1. Spin Dynamics in Nanostructures (J. J. Rhyne)**

The interest in dynamic processes, in particular magnetic excitations, as the dimensions of a specimen are reduced to the nanoscale is currently creating intense scientific interest. This interest ranges from fundamental questions about the form of the exchange interaction and resulting magnon dispersion (Heisenberg, Ising, or a modification) to lifetime and linewidth broadening effects. This is an important area of nanoscale science that will seriously strain the intensity/resolution capabilities of neutron techniques to provide relevant answers. Many of the studies will also benefit from polarized beam techniques. The hybrid spectrometer, HYSPEC, proposed for the SNS plays a pivotal role in the investigation of inelastic processes in nanostructures.

Present interest in magnetic nanoscale materials is in two primary areas – thin films and superlattices and in true magnetic nanocomposites for which nanoscale magnetic clusters are precipitated in a non-magnetic (often amorphous) carrier. Also materials can be prepared where isolated nanosize clusters are formed in the deposition process and can be compacted with resulting changes in the interparticle interactions. The determination of spin dynamics in nanomagnetic materials requires both extremely high beam intensity (partly because of the small sample quantities readily available) and also frequently polarized beam analysis to distinguish the magnon branches from other competing interactions. Spin excitations of mixed ferromagnetic and antiferromagnetic character may be observed requiring measurement of both spin-flip and non-spin flip cross sections to properly interpret the results. A wide range of available energy resolutions, largely decoupled from the  $q$  resolution, as available with HYSPEC will be of tremendous advantage in studying lifetime effects as critical dimensions are reduced.

A conventional ferromagnet exhibits collective excitations with dispersion at long wavelengths (low  $q$ ) given by  $E = Dq^2 + \Delta$ , where  $\Delta$  is an energy gap usually associated with a magnetic anisotropy impeding the excitation of a spin wave. The spin stiffness parameter,  $D$ , is directly related to the exchange constant. This dispersion relation is modified in a nanoparticle system leading to finite-size quantization gaps introduced into the spectrum as the particle size is reduced. A simple “particle in a box” analogy for spin waves places a lower limit on the wave vector ( $q = 2\pi/d$ ) where  $d$  is the particle size and introduces discrete energy levels with finite gaps in the spin-wave spectrum given approximately by  $\Delta_{sw} = D \pi^2/d^2$ . These gaps vanish in large particles, and the spin wave spectrum exhibits conventional dispersion  $E = Dq^2$ .

Hendriksen et al.<sup>2</sup> have calculated the spin-wave spectrum of Heisenberg spin clusters of varying size for clusters ranging from 9 to 749 spins corresponding to nanoparticles of sizes from approximately 7 Å to 32 Å and included both bcc and fcc lattice arrangements. Their results yield a dispersive spin-wave energy with finite-size gaps that vary quadratically with the size of the cluster. For large spin clusters, the gaps are relatively small (e.g. 30K (3 meV) for the 749-spin cluster) but grow to 140K for the 9-spin cluster. Accompanying the formation of the finite-size gaps is a smearing of the wavevector  $q$ , resulting from the abrupt transition from finite spin  $S$  inside a cluster to 0 outside, which is most pronounced for the smallest clusters. One remarkable result from the calculation is that there is no softening in the spin wave energies; in fact the highest state in the 683-spin cluster lies higher than the maximum bulk spin wave energy. The occurrence of the finite-size gaps also modifies the Bloch  $T^{3/2}$  form of the low-temperature magnetization producing a power law dependence  $M(T) = M(0) [1 - BT^\alpha]$ , with  $\alpha \approx 2.0$  for a 20 Å cluster and down to  $\alpha = 1.5$  for an infinite size cluster.

The pioneering studies of excitations in nanoparticles were done by Hennion et al.<sup>3</sup> on approximately 20 Å Fe in an alumina substrate. They found a dual dynamical system consisting of a longitudinal mode corresponding to spin relaxation and a semi-transverse mode reflecting the spin fluctuations. These modes merged into a single isotropic mode at high  $T$  with a temperature-independent fluctuation time they related to the spin anisotropy of individual particles. Subsequently, in a system with larger Fe particles ( $\approx 50$  Å)<sup>4</sup>, they observed the evolution of the fast dynamic magnetization component from a quasi-elastic lineshape into an inelastic lineshape at low temperatures reflecting damped spin waves. Antiferromagnetic spin fluctuations in  $\approx 150$  Å nanoparticles of hematite were studied by Hansen et al.<sup>5</sup> who derived the superparamagnetic spin relaxation time from an analysis of the quasi-elastic linewidth and also were able to distinguish the energies of the intraparticle collective excitations.

In the area of spin dynamics in thin films and superlattices the feasibility of these studies has been demonstrated by Schreyer et al.<sup>6</sup> in their study of a superlattice of  $[Dy_xY_y]_m$ .

<sup>2</sup> P.V. Hendriksen, S. Linderorth, and P.-A. Lindgard, Phys. Rev. B, **48**, 7259 (1993).

<sup>3</sup> M. Hennion, C. Bellouard, I Mirebeau, J.L. Dormann, and M. Nogués, Europhys. Lett. **25**, 43 (1994).

<sup>4</sup> M. Hennion, C. Bellouard, I. Merebeau, J.L. Dormann, and R. Ober, J. Appl. Phys. **75**, 5900 (1994)

<sup>5</sup> Mikkel F. Hansen, Franz Bodker, Steen Morup, Kim Lefmann, Kurt N. Clausen, and Per-Anker Lindgard, Phys. Rev. Letters **79**, 4910 (1997).

<sup>6</sup> A. Schreyer, T. Schmitte, R. Siebrecht, P. Bodeker, H. Zabel, S. H. Lee, R. W. Erwin, C. F. Majkrzak, J. Kwo and M. Hong, J. Appl. Phys. **87**, 5443 (2000).



This system has helical spin order and thus the origin of the spin wave branches is at magnetic-only reflections at incommensurate lattice positions. The magnetic reflections are divided into two sets of satellites on either side of corresponding c-axis nuclear reflections. Thus the total spectral weight is split between branches from each reflection. In addition to the branches from the multiple incommensurate satellite positions, the magnetic coherence across bilayers of the superlattice produces multiple branches from each magnetic satellite separated in  $q$  by  $2\pi/\Gamma$ , where  $\Gamma$  is the bilayer thickness. Existing spectrometers do not have sufficient resolution/intensity trade-off to allow the separation of these multiple branches, and thus the published data are an average over the respective superlattice harmonic branches. A much more intense neutron source combined with a spectrometer such as HYSPEC is anticipated to provide sufficient intensity at the necessary resolution to separate the harmonic spin-wave branches.

The significant intensity advantages offered by HYSPEC combined with full polarization analysis, and highly flexible control over resolution should make this instrument unequalled for the study of magnetic excitations in nanoscale magnetic materials.

### 2.1.2. Nanoscale Features of Functional Materials (V. Kiryukhin)

The drastically enhanced electronic and magnetic responses occurring in complex functional materials as a result of inhomogeneity on a microscopic length scale have recently attracted significant attention. Both fundamental properties, and enhanced materials characteristics potentially useful for industrial applications are currently being actively investigated. During the last 5 years, it has become clear, for example, that nanoscale inhomogeneities are intrinsic to a number of important oxide systems, such as superconducting cuprates<sup>7</sup>, magnetoresistive manganites<sup>8</sup>, and lead-based relaxor ferroelectrics.<sup>9</sup> Also, understanding and controlling the giant structural, optical, and magnetic responses of inhomogeneous materials holds great potential for the creation of technologically advanced consumer products.

Some of the most important systems discussed above exhibit nanoscale magnetic inhomogeneities. In magnetoresistive manganites, for example, nanoscale magnetic inhomogeneities play the crucial role in the so-called Colossal Magnetoresistance (CMR) effect.<sup>10</sup> While it is known that nanoscale magnetic regions exist in these materials, the structural and magnetic properties of these regions remain largely uncharacterized.<sup>10,11</sup> To understand the physics of the CMR effect, and to guide future work for the synthesis of materials with enhanced magnetoresistive properties, it is crucial to determine the magnetic and structural properties of the inhomogeneous states realized in these materials.

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<sup>7</sup> Lang K.M., Madhavan V., Hoffman J.E., Hudson E.W., Eisaki H., Uchida S., Davis J.C., Nature 415, 412 (2002)

<sup>8</sup> E. Dagotto, T. Hotta, and A. Moreo, Phys. Rep. 344, 1 (2001).

<sup>9</sup> P. M. Gehring, S.-E. Park, and G. Shirane, Phys. Rev. Lett. 84, 5216 (2000)

<sup>10</sup> P. Dai, J. A. Fernandez-Baca, N. Wakabayashi, E. W. Plummer, Y. Tomioka, and Y. Tokura, Phys. Rev. Lett. 85, 2553 (2000); C. P. Adams, J. W. Lynn, Y. M. Mukovskii, A. A. Arsenov, and D. A. Shulyatev, Phys. Rev. Lett. 85, 3954 (2000); T. Y. Koo, V. Kiryukhin, P. A. Sharma, J. P. Hill, and S-W. Cheong, Phys. Rev. B 64, 220405(R) (2001)

<sup>11</sup> V. Kiryukhin, T. Y. Koo, A. Borissov, Y. J. Kim, C. S. Nelson, J. P. Hill, D. Gibbs, and S-W. Cheong, Phys. Rev. B 65, 094421 (2002)

Another class of experimental systems that has recently attracted significant attention are doped magnetic semiconductors, such as Mn-doped GaAs and InAs, and Co-doped ZnO and TiO<sub>2</sub>.<sup>12,13</sup> The recent claims<sup>13</sup> of synthesis of room-temperature magnetic semiconductors have generated a significant controversy. It is becoming clear now, that in many cases the prepared systems are actually very fine mixtures of non-magnetic semiconductors (e.g., GaAs or InAs) and ferromagnetic metals (e.g., MnAs or MnSb). Physical properties drastically evolve when the mixed systems vary from complete solid solution to macroscopically phase-separated materials.<sup>14</sup> Some of these systems exhibit very large values of magnetoresistance.<sup>15</sup> A number of these materials can now be synthesised in the bulk form. In order to understand this intriguing behavior, it is essential to characterize the microscopic properties of these materials, with special attention paid to the nanoscale magnetism. In this case, as well as in the CMR manganites discussed above, characterization of both static and dynamic magnetic properties will be of great importance. In particular, the dynamic magnetic properties of the nanoscale regions are expected to be significantly different from the corresponding bulk systems. In fact, drastic changes in the lattice dynamics properties have recently been observed in relaxor ferroelectrics,<sup>9</sup> which can be considered a non-magnetic analogue to the systems described here.

Polarized neutrons will, undoubtedly, be one of the most effective tools to study the nanoscale magnetism in these, and related, systems. A very important factor underlying the usefulness of this probe is that magnetic signals from systems inhomogeneous on nanoscale are both delocalized in the reciprocal space, and spread in energy, and are, therefore, weak. In addition, the nonmagnetic background is typically strongly enhanced in such systems. With the proposed spectrometer (HYSPEC) it would be possible to successfully separate diffuse magnetic signals from the background, such as multiple Bragg scattering, phonons, and incoherent scattering due to isotopic disorder. The polarization analysis will be of crucial importance.

### 2.1.3. Anomalous Phonon Behavior (S. Shapiro, G. Shirane)

It has long been known that structural phase transformations occurring in materials such as ferroelectrics are driven by a lattice vibrational mode whose frequency tends to zero at the transformation temperature. This so-called 'soft' mode usually occurs at a well defined wavevector in a particular optic or acoustic phonon branch and is frequently accompanied by a 'central' peak, i.e. divergent elastic scattering. The anomalies associated with the soft mode result in very anisotropic dispersion curves. Recent work on ferroelectrics like PZT and PMN<sup>9</sup> and on shape memory alloys such as Ni-Al, Ti-Pd, and Ni<sub>2</sub>MnGa have demonstrated the need for good wave-vector resolution and for

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<sup>12</sup> T. Hayashi, Tanaka M, Nishinaga T, Shimada H, Tsuchiya H, Otuka Y., J. Cryst. Growth 175, 1063 (1997)

<sup>13</sup> M. L. Reed, El-Masry N. A., Stadelmaier H. H., Ritums M. K., Reed M. J., Parker C. A., Roberts J. C., Bedair S. M., Appl. Phys. Lett. 79, 3473 (2001); Y. Matsumoto, Murakami M, Shono T, Hasegawa T, Fukumura T, Kawasaki M, Ahmet P, Chikyow T, Koshihara S, Koinuma H., Science 291, 854 (2001)

<sup>14</sup> Y. Shon, Young Hae Kwon, Deuk Young Kim, Xiangjun Fan, Fu D, Tae Won Kang, Jap. J. Appl. Phys. 40, 5304 (2001); S-W. Cheong, unpublished. See, also, "Structural Inorganic Chemistry" A. F. Wells, Fifth edition, (Oxford University Press, 1984), and "Physics of Ferromagnetism" S. Chikazumi, (Oxford University Press, 1997)

<sup>15</sup> H. Akinaga, Mizuguchin M, Ono K, Oshima M., Appl. Phys. Lett. 76, 357 (2000)

minimization of the extraneous elastic scattering from the sample environment. It also makes clear that single crystals are necessary. Most often these crystals are grown explicitly for neutron scattering experiments and tend to be small. Focussing of the incident beam is therefore vital to assure the maximum number of neutrons impinging on the sample; a requirement met by the proposed HYSPEC instrument. A sample stage accepting broad range of sample environment devices, combined with the flexibility to define the sample scattering volume by using the collimators and beam definers, and, therefore, efficiently suppress the incoherent background, is another crucial advantage for studying the coherent (*eg* phonon) scattering from single crystals offered by HYSPEC.

#### 2.1.4. Complex Phases in the Intermetallic Alloys (C. Stassis)

The proposed HYSPEC spectrometer will be a world-class instrument with polarization analysis capability, a feature that makes it a unique instrument among those to be installed at SNS. Actually, the capability of using polarized neutrons is essential in practically any detailed study of the magnetic properties of condensed matter systems. Such studies extend from the determination of the magnetic form factor to a detailed analysis of magneto-vibrational scattering studies, and provide invaluable information about the magnetic properties and, most importantly, the interactions between magnetic and other excitations in condensed matter systems. Currently though, only for one of the reflectometers planned for the SNS is a simple polarized neutron capability envisaged. Polarization analysis capability of the instrument is of particular importance for the study of complex phases. These phases exhibit complicated arrangements of various interacting degrees of freedom (such as spin, orbital moment, charge, etc.), with fascinating physical properties, some of which may be exploited in emerging technologies ranging from high- $T_c$  superconductivity and spin valves to photonic switches and quantum computing. The well-known examples of such systems, presently under intense experimental and theoretical scrutiny, are the various phases of superconducting cuprates and the magnetoresistive manganites.

ROOM TEMPERATURE STRUCTURES OF  $R_5(Si_xGe_{1-x})_4$

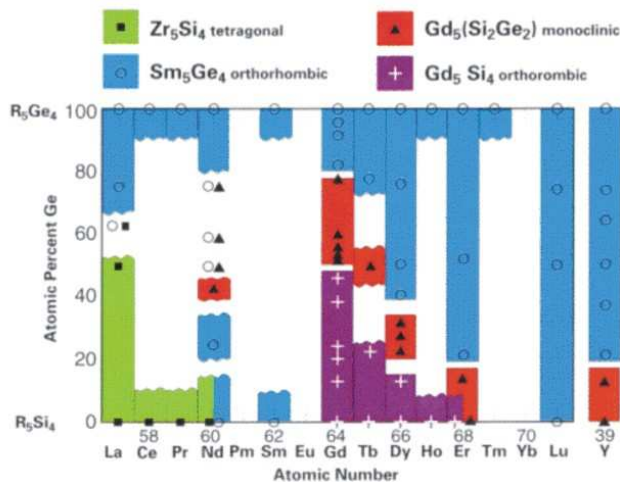


Figure 2.1. The homogeneity ranges and structure types observed in various  $R_5(Si_xGe_{1-x})_4$  systems at room temperature.

Among the complex systems whose physical properties can be exploited in emerging technologies and which therefore have recently attracted considerable attention are the intermetallic compounds of  $R_5(Si_xGe_{1-x})_4$  family. This family was discovered over thirty years ago<sup>16</sup>, and has recently opened up an unprecedented opportunity to solve the century-old problem of the intrinsic

<sup>16</sup> F. Holtzberg, R.J. Gambino, T.R. McGuire, J. Phys. Chem. Solids **28**, 2283 (1967).

relationships between the chemical composition, atomic structure and properties of metallic materials. These compounds exist in nearly every R-Si-Ge system, and the distribution and room temperature crystallography of the  $R_5(Si_xGe_{1-x})_4$  phases is illustrated in Figure 2.1.

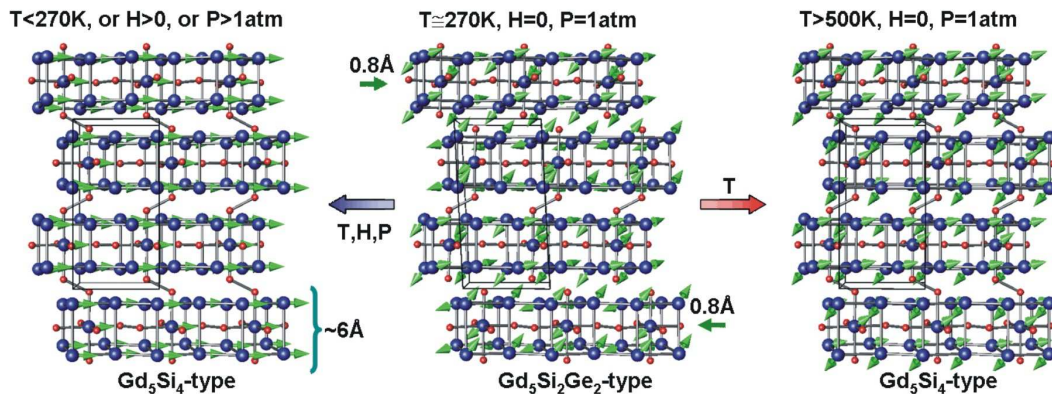


Figure 2.2. The schematic of the coupled magnetic-crystallographic transformation in the  $Gd_5(Si_2Ge_2)$  compound, which near  $\sim 270$  K may be triggered by any of the three thermodynamic variables: temperature, magnetic field and pressure (left). The schematic of the crystallographic-only temperature induced transformation, which occurs between  $\sim 500$  and  $800$  K (right). Gd atoms are indicated using large blue spheres, and Si(Ge) atoms are shown as small red spheres. One of the sub-nanometer thick slabs is highlighted by a bracket. Green arrows indicate the directions in which the slabs move during crystallographic phase changes.

The crystal structures of the  $R_5(Si_xGe_{1-x})_4$  phases consist of 36 atoms per unit cell distributed among 6 to 9 independent crystallographic sites.<sup>17</sup> These alloys exhibit a number of diverse and unique properties<sup>18</sup> associated with both their naturally layered crystal structures and the combined magnetic-crystallographic transformations at low temperatures, driven by a reversible breaking and reforming of specific covalent Si(Ge)-Si(Ge) bonds (Fig. 2.2, left). The crystal structures change via a martensitic-like collective shear movement of sub-nanometer thick slabs by as much as  $1.1 \text{ \AA}$  and are easily affected by magnetic field, temperature, and pressure. The transitions are accompanied by a giant magnetocaloric effect, a colossal magnetostriction, and a giant magnetoresistance, suggesting many possible technological applications in sensors and energy-transforming devices through intelligent manipulation of the phase transformation by composition, applied fields, temperature, and pressure.

For the most part, identical crystallographic transition also occurs at high temperature in the paramagnetic state (Fig. 2.2, right) when the alloy stoichiometries are near critical (i.e. those where compositional variations induce a crystallographic phase change). X-ray powder diffraction measurements indicate that both the low-temperature magnetically ordered and the high-temperature magnetically disordered orthorhombic  $Gd_5Si_4$ -type phases are the same. Preliminary first principles calculations<sup>19</sup> indicate, on the other

<sup>17</sup> V.K. Pecharsky, K.A. Gschneidner, Jr., *J. Alloys Compd.* **260**, 98 (1997); W. Choe, V.K. Pecharsky, A.O. Pecharsky, K.A. Gschneidner, Jr., V.G. Young, Jr., G.J. Miller, *Phys. Rev. Lett.* **84**, 4617 (2000).

<sup>18</sup> V.K. Pecharsky and K.A. Gschneidner, Jr., *Adv. Mater.* **13**, 683 (2001).

<sup>19</sup> V.K. Pecharsky, G. Samolyuk, V.P. Antropov, A.O. Pecharsky, and K.A. Gschneidner, Jr., *J. Solid State Chem.* (Submitted; Presented at the 23<sup>rd</sup> Rare Earth Research Conference, UC Davis, CA, July 13-18, 2002).

hand, that the high temperature phase transition may be an order-disorder transformation, in which Si and Ge atoms are redistributed among their respective lattice sites. This crystallographic phase change has a far-reaching effect on the magnetic properties of the material, as illustrated in Fig. 2.3.

Only systematic neutron scattering studies as a function of composition, temperature, magnetic field, and pressure can provide a detailed understanding of the various phases of these systems, the magnetic-crystallographic transformations and their origin. For such detailed studies, the polarization analysis capability of HYSPEC will be an invaluable tool, since it is essential to establish the origin (magnetic or nuclear) of a large number of peaks observed in the elastic and inelastic neutron scattering studies of these materials.

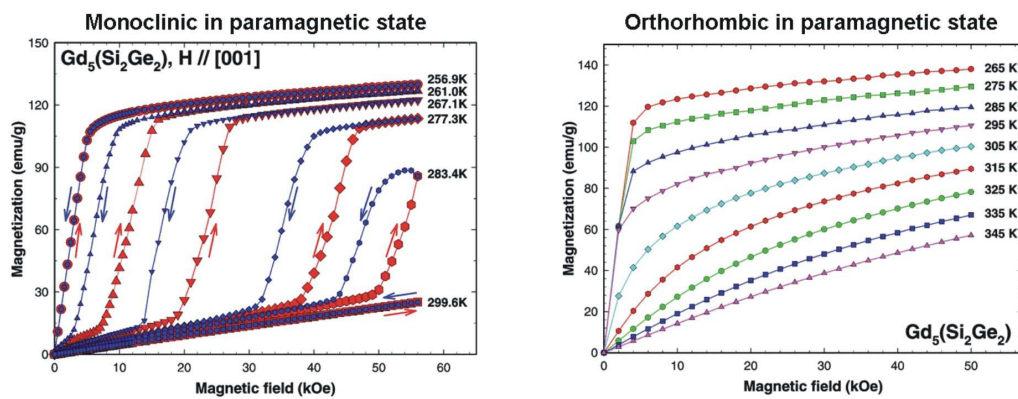


Figure 2.3. The magnetic behavior of two different polymorphs of the  $Gd_5(Si_2Ge_2)$  compound. The monoclinic  $Gd_5(Si_2Ge_2)$ -type structure with half of the interslab bonds undergoes a first order magnetic-martensitic transformation during isothermal magnetization (left). The orthorhombic  $Gd_5Si_4$ -type structure with all interslab bonds displays a conventional second order paramagnetic-ferromagnetic transformation.

Such detailed studies, combined with first principle calculations, are essential for a fundamental understanding of the fascinating properties of these compounds (such as the magnetocaloric effect). The proposed instrument at the high intensity SNS facility is the ideal tool for such detailed investigations.

## 2.2. Correlated Phases in Many-Electron Systems (I. Zaliznyak, J. Tranquada)

The ground states of many-electron systems with spin, orbital and/or charge/valence degeneracy often exhibit non-trivial arrangements of these degrees of freedom which lead to many fascinating physical properties. Recently much attention has been paid to exploring the charge and/or orbital-ordered phases in transition metal oxides such as the superconducting cuprates and magnetoresistive manganites.<sup>20</sup> Understanding the nature and origin of these phases is of both fundamental importance and technological interest. Neutron scattering is the most informative and least perturbing experimental way of providing information on the correlated structural distortions and/or magnetic correlations in the charge/orbital/spin-ordered phases. Among the unique features inherent to the neutron scattering approach is that it provides both good energy and wavevector resolution, which permits accurate discrimination between the static and

<sup>20</sup> J. Zaanen, Science **286**, 251 (1999)

dynamic correlations and allows separate characterization of the corresponding correlation ranges. Examples where this is of crucial importance are the recent observations of stripe liquid phases in the doped layered nickelates,<sup>21</sup> incommensurate dynamical correlation in the cuprate superconductors<sup>22</sup> and characterization of dynamical slow-down in the course of the spin-glass freezing transition in the half-doped cobaltate  $\text{La}_{1.5}\text{Sr}_{0.5}\text{CoO}_4$ .<sup>23</sup> Such capabilities would also provide an excellent opportunity for studying other diverse glassy and short-range-ordered systems and the glass transformations in both “hard” and “soft” condensed matter systems.

A spectrometer, optimized for studies of the short- and long-range static and dynamic correlations in single crystals should be designed to have both small elastic and a negligible inelastic background, a symmetric and well-reproduced resolution function (permitting a straightforward and reliable (de)convolution procedure) and have a polarization analysis capability to distinguish between structural and magnetic scattering. Equally important, it should provide complete and continuous coverage of a significant volume in the reciprocal space of the crystal with both energy and wavevector resolution easily adaptable to the type of the problem studied. Finally, it is essential that such an instrument be easily equipped with a variety of sample environments since definitive insight into the nature of many-electron correlated phases is often obtained by studying how they are affected by changes in external magnetic field, temperature, pressure, etc. As it is evident from Section 3, the proposed HYSPEC spectrometer is designed to both provide superior performance and to address these concerns.

### 2.3. Strongly Correlated Electrons

#### 2.3.1. New Challenges for Neutron Scattering (G. Lander, S. Nagler)

Strongly correlated electron systems, from heavy-Fermions to high- $T_c$  and to compounds exhibiting giant magneto-resistance effects, has added a new class of materials to those with which we are familiar. Of crucial significance in these materials are the role of electron correlation energies and the interaction of the lattice with the spin degrees of freedom. Unlike the BCS superconductors in which vibrational degrees of freedom (the phonons) play a key role in mediating superconductivity, the new phenomena are classified as having a range of interactions, with the dominant one often difficult to identify.

Neutron inelastic scattering is the single most important probe for unraveling the energetics and spatial dependencies of these interactions. At the same time, we have to be able to separate interactions that are electronic from those that are vibrational. This requires polarized neutrons, and very often polarization analysis. We may demonstrate the argument by invoking the pioneering work by Axe and Shirane<sup>24</sup> on the vibrational spectra of  $\text{Nb}_3\text{Sn}$  above and below  $T_c$ . These experiments, performed in the 1970s, used unpolarized neutrons. Because superconductivity in BCS materials are dominated by

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<sup>21</sup> S.-H. Lee, J. M. Tranquada, K. Yamada, D. J. Buttrey, Q. Li, S.-W. Cheong, Phys. Rev. Lett. **88**, 126401 (2002)

<sup>22</sup> N. Ichikawa, S. Uchida, J. M. Tranquada, T. Niemöller, P. M. Gehring, S.-H. Lee, J. R. Schneider Phys. Rev. Lett. **85**, 1738 (2000)

<sup>23</sup> I. Zaliznyak, J. P. Hill, J. Tranquada, R. Erwin, Y. Moritomo, Phys. Rev. Lett. **85**, 4353 (2000)

<sup>24</sup> J. D. Axe and G. Shirane, Phys. Rev. Lett. **30**, 214; Phys. Rev. B **8**, 1965 (1973)

vibrational energies there has never been any doubt that the measurements were of phonons. However, if we think today of the superconductivity of UPd<sub>2</sub>Al<sub>3</sub> or of high-T<sub>c</sub> materials, that question is much harder to answer. In both UPd<sub>2</sub>Al<sub>3</sub><sup>25</sup> and high-T<sub>c</sub> materials<sup>26</sup> full polarization analysis has proved of enormous value in separating the electronic and lattice effects.

Another challenge to our understanding of the strongly correlated electron systems is presented by Ruthenates and other 4d and 5d based Ruddlesden-Popper and pyrochlore structures. The typical energy scales in these systems are a few meV, and they tend to show odd incommensurate fluctuations similar to those in high-T<sub>c</sub> type materials, as well as quantum critical behavior in the doped materials. It would be very useful to study the fluctuations in these materials using fully polarized inelastic scattering.

We need to continue to develop the technology of polarized beams and polarization analysis (PA), so that these experiments can extend over a wider range of energy than presently available and not be so demanding in terms of intensity. Very large crystals are presently required to map out excitations in full PA,<sup>27</sup> which means that the technique cannot be generally used. An instrument at the SNS will therefore open a completely new field of endeavor. Not just to be able to perform PA on selected excitations, but, more importantly, to construct  $S(\mathbf{Q}, \omega)$  maps of spin-flip and non-spin-flip intensity.

Furthermore, efforts in three-dimensional polarization analysis, now done almost exclusively with the spherical neutron polarimeter at the ILL, can often make unambiguous identification of magnetic configurations<sup>28</sup> and need to be implemented on a wider scale. Its extension into inelastic scattering is just beginning.<sup>29</sup> Many surprises in our understanding of magnetism, and in defining precise interactions, will emerge with the use of polarized neutrons.

#### **2.4. High-T<sub>c</sub> Superconductors and Advanced Polarization Analysis using TAS and TOF spectrometers (L.-P. Regnault)**

Much of the present condensed matter research is devoted to understanding the physics of "strongly correlated electronic systems". This class of systems encompasses a large variety of physical situations: un-conventional "d-wave" superconductivity in high-T<sub>c</sub> superconductors (LSCO, YBCO...) or spin-ladder cuprates (Sr<sub>14</sub>Cu<sub>42</sub>O<sub>41</sub>...), un-conventional "p-wave" superconductivity (Sr<sub>2</sub>RuO<sub>4</sub>, UGe<sub>2</sub>, CePd<sub>2</sub>Al<sub>2</sub>...), charge-ordered materials (NaV<sub>2</sub>O<sub>5</sub>, Sr<sub>14</sub>Cu<sub>24</sub>O<sub>41</sub>, LaNiO<sub>4+y</sub>...), spin-Peierls materials (CuGeO<sub>3</sub>, FeOCl, Pb[Cu(SO<sub>4</sub>)(OH)<sub>2</sub>]...), exotic spin dynamics in quantum-chain systems (J<sub>1</sub>-J<sub>2</sub> systems, alternating chains, Haldane-gap chains, dimer systems, magnetization-plateau systems...), highly frustrated systems (kagome, J<sub>1</sub>-J<sub>2</sub>-J<sub>3</sub> honeycomb, pyrochlore...), etc.

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<sup>25</sup> N. Bernhoeft et al., Phys. Rev. Letters **81**, 4244 (1998)

<sup>26</sup> H. Fong et al., Phys. Rev. B **61**, 14773-14786 (2000)

<sup>27</sup> R. Caciuffo et al., Phys. Rev. B **59**, 13892 (1999)

<sup>28</sup> S. H. Lee et al., Phys. Rev. B **60**, 10405 (1999); A. Hiess et al., Phys. Rev. B **64**, 134413 (2001)

<sup>29</sup> See article by Caciuffo et al. in ILL Annual report 2001



The physics which is involved in all these systems may be understood from the competition of different degrees of freedom: spin, orbit, charge and lattice distortion. The understanding of mechanisms at the origin of exotic properties is only possible if one can

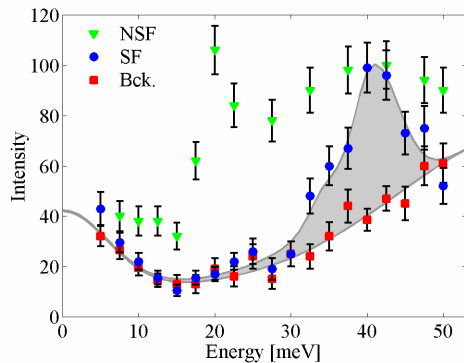


Figure 2.4: Energy scan through the antiferro-magnetic zone center at  $\mathbf{Q}=(1.5,0.5,1.7)$ : non-spin-flip (green circles) and spin-flip (blue circles) intensity, and background position  $\mathbf{Q}=(1.8,0.6,1.7)$  (red squares) for an incident polarisation parallel to  $\mathbf{Q}$  (spin-flip channel). The energy dependence of the background is due to the increased counting time at higher incident energies. The shaded area illustrates the magnetic signal peaking at the resonance position of 41 meV.

determine accurately and unequivocally the wave vector and energy dependencies not only of the "standard" correlation functions (i.e. those coupling identical degrees of freedom :  $\langle\text{spin-spin}\rangle$ ,  $\langle\text{orbit-orbit}\rangle$ ,  $\langle\text{displacement-displacement}\rangle\dots$ ), but also the "hybrid" correlations functions coupling different degrees of freedom ( $\langle\text{spin-orbit}\rangle$ ,  $\langle\text{spin-displacement}\rangle$ ,  $\langle\text{orbit-displacement}\rangle\dots$ ). To our knowledge, the only way to solve this problem is to measure the magnetic-magnetic (MM), nuclear-nuclear (NN) and magnetic-nuclear (interference) terms using the inelastic polarized neutron scattering in conjunction with a powerful polarization analysis technique.

The best known polarization analysis technique is the so-called "longitudinal polarization analysis" (LPA) method invented a long time ago by Shull, Moon, Riste and Kohler.<sup>30</sup> The LPA is invaluable to obtain separately the magnetic and structural

contributions, or the various magnetic components at a given scattering vector. We have recently used the LPA on IN22 at ILL to determine directly the magnetic excitation spectrum in the high-Tc compound  $\text{YBCO}_{6.85}$  (Fig. 2.4)<sup>31</sup> and in ladder material  $\text{Sr}_{14}\text{Cu}_{24}\text{O}_{41}$ .<sup>32</sup> The advantage of using a polarized beam versus an unpolarized one is clearly demonstrated in Fig. 2.4. The magnetic response is superposed onto a series of more or less well-controlled structural features (phonons, "braggons", "spurions"...), which render the determination highly uncertain. The same scan performed with a polarized beam allows a very precise determination of the magnetic contributions (in particular the resonant peak at 41 meV and the IC dynamic correlations existing between 25 meV and 41 meV). The "normal" method would have consisted in performing constant-energy scans at different energies to determine both the signal and the background.

Some years ago (in the early 80's), the LPA was successfully used on IN12 at ILL to demonstrate the relevance of soliton-type non-linear excitations in the quasi-1D antiferromagnet TMMC.<sup>33</sup> In particular, the use of polarization analysis was fundamental

<sup>30</sup> R. M. Moon, T. Riste, and W.C. Koehler, Phys. Rev. **181**,920 (1969)

<sup>31</sup> H. M. Ronnow, L.P. Regnault, C. Ulrich, B. Keimer, P. Bourges, and Y. Sidis ILL Annual Report 2000

<sup>32</sup> L. P. Regnault et al, unpublished

<sup>33</sup> J.P. Boucher et al., Europhys. Lett. (1985)



to determine unequivocally and separately the contribution  $S^{\parallel}(\mathbf{Q}, \omega)$ , directly related to the solitons, and  $S^{\perp}(\mathbf{Q}, \omega)$ , related to the inter-soliton spins, Fig. 2.5. With un-polarized neutrons, the method to separate both contributions would have consisted in measuring the  $Q$ -dependence of the response, which is problematic if one contribution is much smaller than the other. A recent example is measurement of the SF and NSF contributions in  $\text{CuGeO}_3$ , a prototype spin-Peierls system, which allowed a spectacular determination of all the magnetic (bound states, continuum...) and phonon modes, and the double-gap structure of the magnetic excitation spectrum.

The LPA method can be transposed to TOF machine. At least there is no conceptual interdiction, although the practical realization may not be simple. As important it has been, the LPA method is still a relatively "old" and "rustic" method. Indeed, LPA only

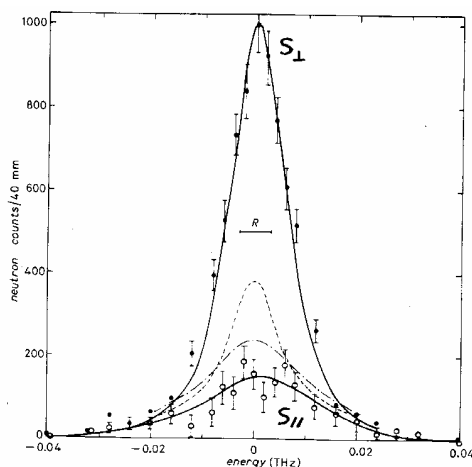


Figure 2.5: Energy spectra of magnetic fluctuations observed in directions parallel and perpendicular to the external field at  $\mathbf{Q}=(1.4,0,1.006)$ . R represents the instrumental resolution. The full lines are theoretical prediction of the flipping model.

recovers one part of the information. Because the incident polarization direction is selected by applying a magnetic field on the sample, only a single projection of the polarization vector after scattering can be determined. In the last decade an important effort has been made at ILL to develop a new polarization analysis technique, offering the possibility to measure all three components of the final neutron polarization (CRYOPAD concept).<sup>34</sup> The "spherical neutron polarimetry" (SNP) is a new alternative to LPA. It has demonstrated strong capabilities in diffraction, in particular to resolve non-trivial magnetic structures.<sup>35</sup>

By accessing the "off-diagonal" components of the polarization tensor (i.e.  $P_{xy}, P_{xz}, P_{yz}...$ ), the method allows, in principle, to determine the so-called "inelastic nuclear-magnetic interference" (INMI) terms.<sup>36</sup> SNP is a very elegant but difficult method to measure very-

small magnetic or structural **inelastic** contributions through their interferences with the strong ones. Although the method has not yet been demonstrated for INS, the SNP could bring new information for, e.g., the relevance of orbital correlations, "hidden-order", orbital currents in High- $T_c$  cuprates or in heavy-fermion materials ( $\text{URu}_2\text{Si}_2$ , etc). This field of investigation is new for INS and almost all remains to be done.

HYSPEC offers a unique opportunity to develop new polarization analysis techniques at a pulsed spallation source. Of course, a broad-band/broad-angle CRYOPAD adapted to TOF spectrometry has not yet been built (although there is a project and some ideas at ILL). On the other hand, the flexibility of HYSPEC associated with its "hybrid" nature, will make the "mono-detector/narrow beam" SNP method easily adaptable.

<sup>34</sup> F. Tasset, Physica B **156-157**, 627 (1989)

<sup>35</sup> P.J. Brown, J.B. Forsyth, and F. Tasset, Proc. R. Soc. London A **442**, 147 (1993)

<sup>36</sup> M. Blume, Phys. Rev. **130**, 1670 (1963)

### 2.4.1. New Transition Metal Oxides (M. Greven)

Transition metal oxides are highly complex materials with coupled charge, spin, and lattice degrees of freedom. These materials are at the frontier of condensed matter physics since they provide myriad possibilities to discover and study novel fundamental phenomena and phases, and because some of their properties, such as high-temperature superconductivity and colossal magnetoresistance, have potential applications in technology. The properties of these systems are generally found to be highly anomalous and have eluded a huge amount of effort over the last 15 years to describe them within the context of conventional theories. Thus they present a formidable challenge to develop new theoretical concepts toward a deeper understanding of the solid state.

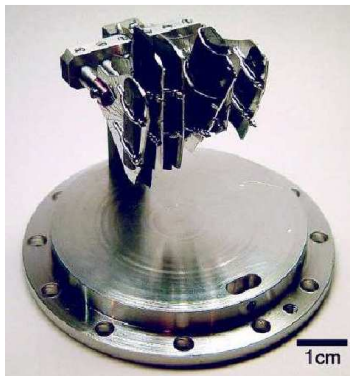


Figure 2.6. A multi-crystal sample of an optimally doped Bi2201.

Neutron scattering plays an invaluable role in materials science and condensed matter physics, as it provides essential structural and magnetic information about new phases of matter and the transitions between them. Such experiments often rely on timely access to sizable, high-quality samples. Over the past few years, we have built a lab at Stanford University to grow some of the most challenging cuprates and manganites for scattering experiments. The center pieces of our crystal growth are three optical floating-zone furnaces which have allowed us, for the first time, to grow sizable crystals of the quantum percolation system  $\text{La}_2(\text{Cu,Zn,Mg})\text{O}_4$ ,<sup>37</sup> and the single-layer bismuth-based superconductor (Bi2201).

A picture of an optimally doped Bi2201 sample with  $T_c$  of 36K is shown in Figure 2.6.

A successful mapping of the antiferromagnetic fluctuations in Bi2201 and related transition metal oxides will be greatly facilitated by the superior neutron flux on the available realistic samples, such as shown in Figure 2.6, and polarized-neutron capabilities of HYSPEC. Quite generally, while the coupling between electrons and phonons is known to be the driving mechanism for Cooper-pair formation in conventional superconductors, its role in the high- $T_c$  superconductors is the subject of intense research efforts.<sup>38</sup> It appears likely that both structural and magnetic degrees of freedom give rise to the fascinating properties of these and related complex oxides, and polarized-neutron capabilities of HYSPEC will help greatly in separating out the two contributions in the relevant energy range.

### 2.5. Quantum Critical Points (R. Osborn)

A quantum critical point is a phase transition in which the temperature at which long-range order is established is suppressed to zero by quantum disorder. This may be induced either externally, e.g. with the application of pressure or magnetic field, or internally through either compositional variations or by increasing disorder. Close to a quantum critical point, the energy scale of critical fluctuations is determined by the temperature which leads to highly unusual scaling of the critical dynamics. Universal

<sup>37</sup> O.P. Vajk et al., Science 295, 1691 (2002).

<sup>38</sup> M. d'Astudo et al., Phys. Rev. Lett., 88 167002 (2002), and references therein.

scaling in  $\omega/T$  has been observed by inelastic neutron scattering in at least two systems believed to be close to quantum critical points,  $\text{UCu}_{5-x}\text{Pd}_x$  and  $\text{CeCu}_{6-x}\text{Au}_x$ . Such experiments are challenging because they require measurements over a wide range of energies. Thus far, the most complete data have been obtained on time-of-flight spectrometers at both reactor and pulsed neutron sources. However, the need for large samples has necessitated the use of systems in which quantum criticality is induced by sample non-stoichiometry rather than by an extreme sample environment. Theoretically, it is important to reproduce this scaling behavior in high-quality single crystals that are stoichiometric so that atomic disorder can be discounted as a contributory factor. For instance, the most reliable examples of quantum phase transitions are in systems such as  $\text{CePd}_2\text{Si}_2$  and  $\text{ZrZn}_2$ , occurring at pressures of 28 kbar and 21 kbar respectively. There is also evidence that metamagnetic transitions in some heavy fermion compounds - commonly occurring in fields of greater than 10 T - may be associated with quantum phase transitions. An instrument with the ability to utilize versatile extreme sample environments, such as HYSPEC, will be especially valuable in investigating quantum phase transitions. Also, the focusing properties of HYSPEC will be vitally important in view of limited sample sizes and volumes.

## 2.6. Geometrically Frustrated Magnets (J. Gardner)

The study of geometrically frustrated magnetic materials<sup>39</sup> has over the past decade resulted in several influential pieces of work<sup>40</sup> in the general area of model magnetism. In these systems, the constraints put on the system by both the local structure and the magnetic interactions generally preclude the occurrence of a long range ordered magnetic state. The phenomenon known as geometric frustration is often displayed in materials containing antiferromagnetically coupled magnetic moments which reside on geometrical units, such as triangles and tetrahedra. The best known example occurs for the two dimensional triangular framework of unidirectional, classical, antiferromagnetically-coupled magnetic moments. In such a system, any two moments can align in a spin-up, spin-down arrangement but the third cannot satisfy both its nearest neighbours simultaneously. In three dimensions systems of corner-sharing tetrahedra, the situation is similar with at least two antiferromagnetic “bonds” frustrated at any one time. The only constraint on the ground state of such a system, is the vector sum of the spins on a frustrated unit (the triangle or tetrahedron) is zero.

In the search for the elusive spin liquid, chemists have synthesized some exotic, magnetically frustrated spin systems. In particular, many new spin  $1/2$  systems have been prepared in the hunt for the Resonant Valence Bond state predicted by Anderson.<sup>41</sup> One

<sup>39</sup> For reviews see *Magnetic Systems with Competing Interactions*, edited by H.T. Diep (World Scientific, Singapore, 1994); A.P. Ramirez, *Handbook of Magnetic Materials*, edited by K. J. H. Buschow, Vol. 13, Chap. 4, p. 423 (Elsevier, Amsterdam, 2001) and *Can. J. Phys.* **79**, (2001).

<sup>40</sup> M. J. Harris, S. T. Bramwell, D. F. McMorrow, T. Zeiske and K. W. Godfrey, *Phys. Rev. Lett.*, **79**, 2554 (1997); A. P. Ramirez, A. Hayashi, R. J. Cava, R. Siddharthan and B. S. Shastry, *Nature*, **399**, 333 (1999); J. S. Gardner, S. R. Dunsiger, B. D. Gaulin, M. J. P. Gingras, J.E. Greedan, R. F. Kiefl, M. D. Lumsden, W. A. MacFarlane, N. P. Raju, J. E. Sonier, I. Swainson and Z. Tun, *Phys. Rev. Lett.*, **82**, 1012 (1999); S. -H Lee, C. Broholm, W. Ratcliff, G. Gasparovic, Q. Huang, T. H. Kim and S. -W. Cheong, *Nature*, **418**, 856 (2002).

<sup>41</sup> P. W. Anderson, *Science*, **235**, 1196 (1987).

possible candidate was  $\text{Sr}_2\text{CaReO}_6$ ,<sup>42</sup> where the spin  $\frac{1}{2}$  Re ions are strongly coupled antiferromagnetically in the face centred cubic lattice. Another antiferromagnetically-coupled system of great interest lately is  $\text{Tb}_2\text{Ti}_2\text{O}_7$ . This co-operative paramagnet does not order magnetically above 17 mK; that is the  $5 \mu_B$ ,  $\text{Tb}^{3+}$  moments continue to fluctuate even at this extremely low temperature. Recently however, we have shown that this system can be driven into a long range ordered state at  $\sim 2$  K with the application of exceptionally high pressures (9 GPa).<sup>43</sup>

For over 5 years now, it has been known that a ferromagnetically-coupled system on a lattice of corner-sharing tetrahedra can also be frustrated. Several compounds enter a disordered magnetic state known as a Spin ice.<sup>44</sup> In these materials ( $\text{Ho}_2\text{Ti}_2\text{O}_7$  and  $\text{Dy}_2\text{Ti}_2\text{O}_7$ , for example) the crystal-field ground state of the rare-earth ion is an Ising-like doublet with magnetic moment ("spin") constrained to a local cubic  $\langle 111 \rangle$  axis. In the context of the cubic lattice symmetry, this constraint frustrates the dominant dipolar interactions in the system and leads to frozen, non-collinear, spin disorder below  $\sim 1$  K. The spin ice state is analogous to the Pauling hydrogen disorder of water ice ( $\text{H}_2\text{O}$ ), with each spin equivalent to a hydrogen displacement vector situated on the mid-point of an oxygen-oxygen line of contact. It is a well-defined magnetic state, intermediate between the paramagnetic state and the much more complex disorder that occurs in spin glasses.

Geometrically frustrated materials typically display diffuse scattering that extends over several Brillouin zones and low energy fluctuating spins. This often makes it difficult to distinguish between the magnetic scattering and the other forms of diffuse scattering. For this reason alone HYSPEC, with its polarisation analysis capabilities will be indispensable to these studies at the SNS. However, it has many other desirable features. The small signal associated with the spin half systems will benefit from the high flux as well as the polarisation capabilities. The large accessible sample space will allow us to study these systems under the extreme conditions (ultra low temperatures and high magnetic field) where unusual phase transitions have been observed.

Finally, many new materials are being grown and will continue to be synthesised by chemists, and these samples are likely to be small due to their complicated chemistry. The high flux, polarisation analysis and the flexibility in this spectrometer will provide us with a very unique instrument for the study of these new magnetic materials.

## 2.7. Quantum Spin Systems (A. Zheludev)

Amazing progress has been made in the field of quantum low-dimensional magnetism in the past twenty years, almost entirely driven by inelastic neutron scattering experiments. The simplest fundamental model systems are by now very well understood. Today the challenge is to learn about more complex phenomena such as the effects of disorder and impurity substitution, spin-lattice interactions and one- and two-dimensional to three-dimensional crossover effects.

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<sup>42</sup> C. R. Wiebe, J. E. Greedan, G. M. Luke and J. S. Gardner, Phys. Rev. B **65**, 144413 (2002).

<sup>43</sup> I. Mirebeau, I. N. Goncharenko, P. Cadavez-Peres, S. T. Bramwell, M. J. P. Gingras and J. S. Gardner, Nature, **420**, 54 (2002).

<sup>44</sup> S. T. Bramwell, M. J. P. Gingras, Science **294**, 1495 (2001).

One example of a new research direction in quantum magnetism is the problem of *random-exchange* spin chains. Consider the case of a  $S=1/2$  quantum spin chain with nearest-neighbor Heisenberg exchange interactions of random magnitude. In the simplest model, a given percentage  $x$  of the bonds are of magnitude  $J_1$ , and the remaining  $(1-x)$  bonds correspond to a coupling strength  $J_2$ , the strong and weak bonds being distributed randomly. For a fixed  $x$  the limiting cases are easy to understand. For  $J_1 \ll J_2$  the chain breaks up into an ensemble of finite-sized clusters: dimers, trimers, tetramers, etc. Each cluster has a *discrete* excitation spectrum, that in a neutron experiment appears as a series of sharp excitations at well-defined energies. For  $J_1=J_2$  the situation is entirely different. In a *uniform* spin chain such as this, the spectrum is an exotic continuum of states with no sharp excitations and a strong wave vector dependence. The question is: how does the spectrum look in the intermediate case of  $J_1 \sim J_2$ ?

To date, the answer is not known, even theoretically. The main reason is that an experimental realization of a model suitable for inelastic neutron experiments has not been available until the recent preparation of the new model compound  $\text{BaCu}_2(\text{Si}_x\text{Ge}_{1-x})_2\text{O}_7$ . Solid solutions with  $0 < x < 1$  are characterized by susceptibility curves that can be fitted to a Bonner-Fisher law with an intermediate value of  $J$  and are expected to be realizations of the  $S=1/2$  random-exchange model. Inelastic neutron scattering experiments on  $\text{BaCu}_2(\text{Si}_x\text{Ge}_{1-x})_2\text{O}_7$  single crystal samples are expected to provide unique insight into the role of disorder in quantum magnets.

Previous work on the  $x=1$  system was carried out on thermal and cold triple-axis instruments at reactor sources as well as on the MARI time of flight instrument at ISIS. It is clear from these measurements that none of these instruments will be fully adequate for the study of the solid solution  $\text{BaCu}_2(\text{Si}_x\text{Ge}_{1-x})_2\text{O}_7$ . First of all, the excitation bandwidth for  $x$  close to unity is expected to be of the order of 150 meV and using a spallation source instrument becomes mandatory if one wants to cover the relevant energy range. At the same time, the small sample size (the largest existing crystals of  $\text{BaCu}_2\text{SiGeO}_7$  are about  $4 \times 4 \times 10 \text{ mm}^3$ ) will require the ability to focus the incident beam to a small spot size; a major feature of HYSPEC. Moreover, the weak and diffuse nature of continuum scattering requires a very low and well-controlled instrument background. Finally, to gain a detailed understanding of the spin dynamics, polarized neutron experiments will be needed. All of these needs will be satisfied by the proposed HYSPEC instrument.

### 3. THE HYSPEC SPECTROMETER

In this section we describe conceptual design, operational principles and performance characteristics of the proposed instrument. A draft of the HYSPEC top-level specifications with detailed and more technical description of the spectrometer components and parameters is attached in Appendix C.

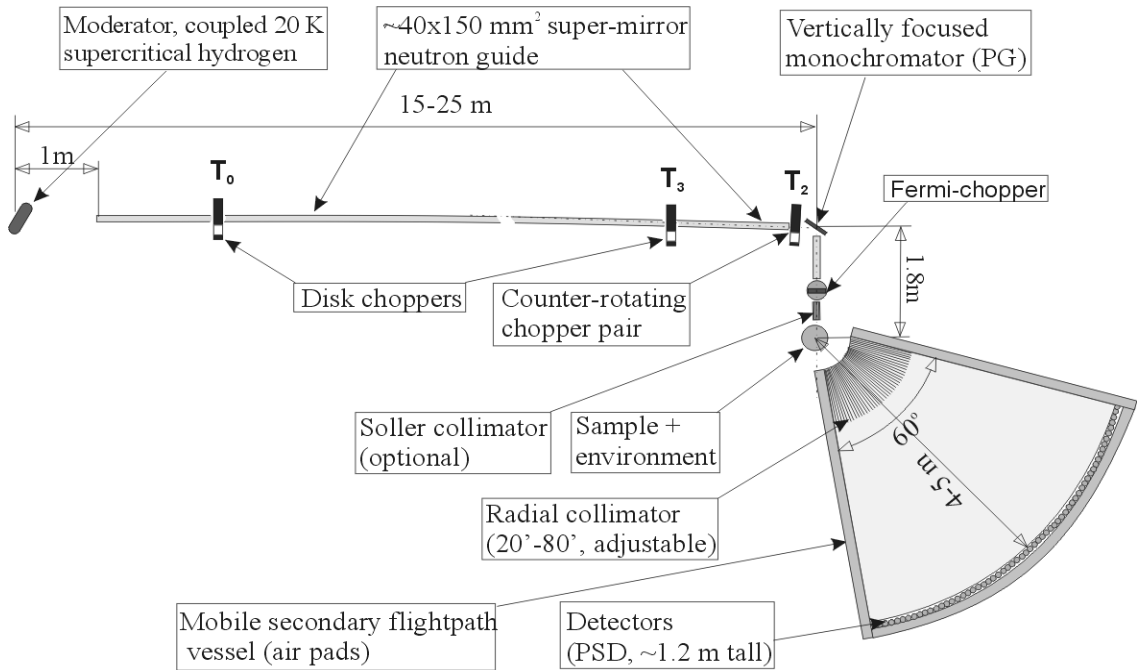


Figure 3.1 Schematic showing HYSPEC's principle elements.

Our primary objective in formulating the design of the HYSPEC spectrometer was that it deliver the highest possible monochromatic flux to few-cm-sized samples over a broad range of thermal and sub-thermal neutron energies [5,90] meV. Additionally, we wanted to develop a design that would (i) minimize beam-related background such as that arising from sample environments, (ii) provide reasonably good (and easily adjustable) energy and scattering vector resolution ( $\delta E/E \sim 0.02 - 0.15$ ;  $\delta Q/Q \sim 0.005 - 0.1$ ), (iii) be readily adapted to polarization analysis, (iv) permit rapid alignment of samples and easy installation of specialized sample environments and (v) allow for straightforward, direct, on-line monitoring and analysis of incoming data. Ultimately these criteria led us to the direct geometry, hybrid concept shown schematically in Figure 3.1 and in a 3-D view on the cover. The instrument main design parameters are summarized in Table I.

**Table I. Instrument Parameters**

Moderator	Coupled, 20K, supercritical H <sub>2</sub>
Incident energy	5 - 90 meV
Energy resolution	0.02 <math>\Delta E/E</math> <math>< 0.15</math> (for elastic scattering) depending on neutron energy and rotation rates of choppers

Q resolution	$\Delta Q/Q \sim 0.005 - 0.1$
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	Segmeted, 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 <sup>2</sup>
Detectors	188 2.5cm diameter position sensitive <sup>3</sup> He tubes. Horizontal pixel resolution 20 min. Vertical pixel resolution 20 min. Horizontal array acceptance: 60°. Vertical array acceptance: $\pm 7.5^\circ$
Sample environment	Will accept all standard sample environment equipment

### 3.1 Primary spectrometer (Monochromator)

Incident neutron energy will be defined by the time of flight in the primary spectrometer. Reflection from the vertically curved monochromator crystal in most cases will only serve to focus the beam onto the sample. In addition, the monochromator will serve in place of the pulse-shaping chopper, cutting the unwanted high-energy tail of the spectral distribution of the incident neutrons, as shown in Figure 3.2. The primary spectrometer is envisioned as consisting of a 20 to 25 meter long 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, Figure 3.1. Whether the guide will be straight or slightly curved is still an open question that will ultimately be resolved by detailed shielding studies. Placed at intervals along the guide would be three disk choppers; the  $T_0$  and frame-overlap choppers - rotating at either the source frequency or a sub-multiple, and a counter-rotating disk chopper pair, rotating at integral multiples of the source frequency. A rotating drum shield containing a vertically-focusing crystal, a beam stop (or, if a straight guide is used, a “get lost” pipe), a vertically tapered guide, a Fermi chopper and a Soller collimator will be placed at the guide’s downstream end. Attached to the shield - and moving with it - would be a conventional sample rotation stage mounted on air pads, with a 2-axes goniometer capable of supporting large, off-center loads. In such an arrangement, neutron energies are determined both by the beam exit angle (as defined by the crystal and the in-shield collimator), and by the phase of rotation of the counter-rotating chopper pair and/or the Fermi chopper relative to the source. Apart from its energy defining function, the crystal - together with the section of vertically tapered

supermirror guide in the drum shield – also has the important function of efficiently focusing the beam at the sample position.

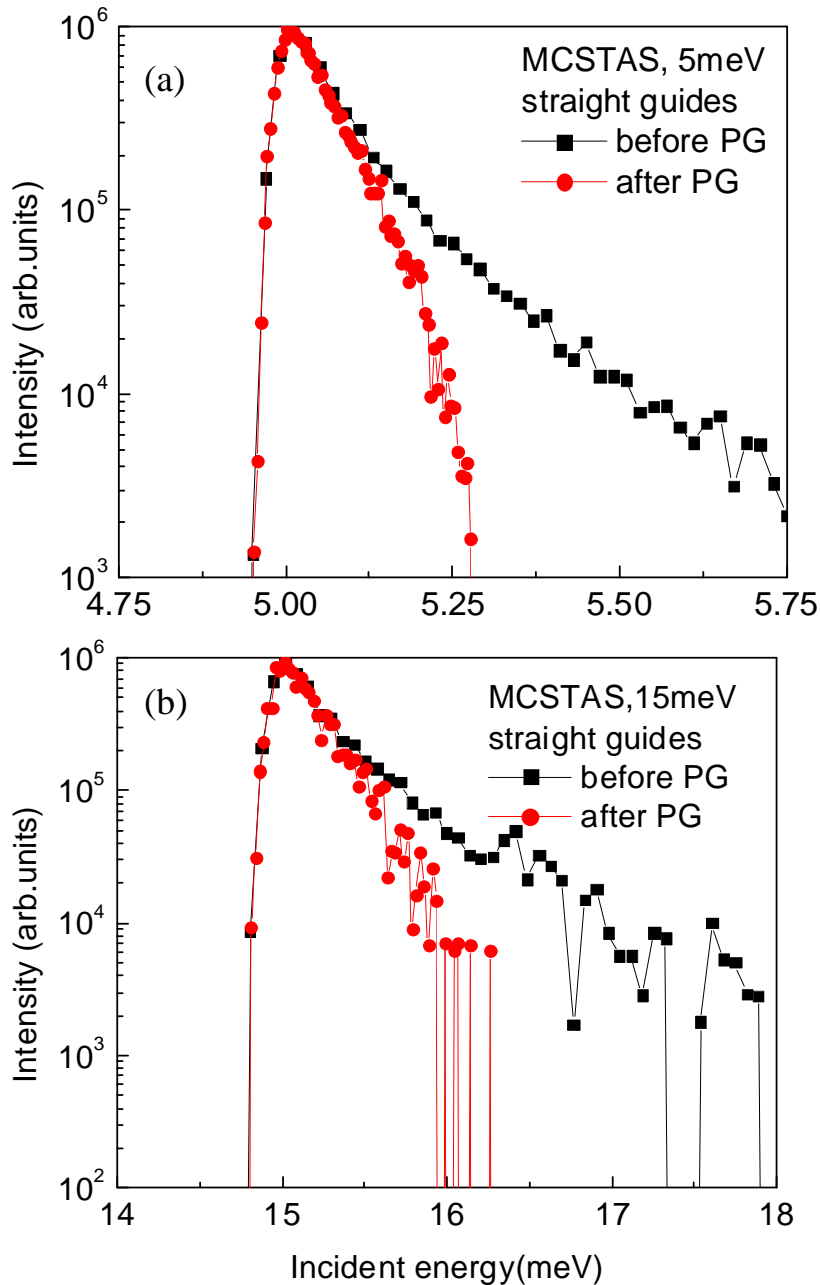


Figure 3.2. Incident neutron spectrum before and after reflection from a PG monochromator: (a)  $E = 5$  meV; (b)  $E = 15$  meV.

Each chopper has a unique role in defining the monochromatic incident beam. The  $T_0$  chopper blocks 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 (shorter wavelength) 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 the main, medium-resolution, high-data-collection-rate mode of operation, the counter-rotating disk choppers  $T_2$  (together with the crystal) will define both 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, it is envisioned that the time width of the sample pulse would 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.

For the focusing crystal, we propose using (for non-polarized applications involving incident neutron energies of 5 meV and higher) individual pyrolytic graphite (PG) plates attached to a segmented GMI-type holder. This arrangement will provide optimal vertical focusing over the entire 5-90 meV neutron energy range. Because a relatively broad horizontal mosaic (probably  $1.0^\circ$ ) will be needed for optimum performance, we plan to use sets of three ZYA grade PG plates stacked with spacers to slightly offset the angles between them. This so-called “fanned arrangement” has been demonstrated to expand the horizontal mosaic but leaves the vertical mosaic (and thus the vertical focusing properties of the crystal) unchanged. At incident neutron energies below 5 meV, where high monochromator scattering angles hamper measurements because of the excessively tight resolution introduced by the PG crystal in a near backscattering geometry and space restrictions, we envision substituting an equivalent crystal composed of fanned plates of fluorinated synthetic mica.

### **3.2 Sample Stage**

As emphasized in the Scientific Objectives Section, it is important for many of the areas of research for which HYSPEC is intended that specialized sample environments can be easily and quickly installed. Because the collimation upstream and downstream of the sample will 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 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. This is another unique feature of HYSPEC.

### **3.3 Secondary Spectrometer (Analyzer/Detector)**

Scattered neutron energy analysis would be done by time-of-flight alone. We propose using a 4.5 meter radius array made up of 188 one-dimensional, position-sensitive, tube-type  $^3\text{He}$  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) interposed between the sample and detectors would restrict their 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  $\pm 7.5$  degrees with respect to the scattering plane. It would 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 detector area would most likely be gas filled and located in a fixed, well shielded housing.

### **3.4 Polarization Analysis**

One of the particularly attractive features of the HYSPEC concept is that it can quickly and easily be adapted to polarization analysis. All that is required is that the focusing crystal used for non-polarized studies be replaced by a crystal that both focuses and polarizes the monochromatic beam incident on the sample and that polarization analyzers be installed between the sample and detectors. The crystal we propose using for polarized applications and the selection of a polarization analyzer will be addressed in the paragraphs that follow.

#### **3.4.1 The Polarizing Crystal**

Polarizing crystals are crystals of ferromagnetic materials with low index Bragg peaks in which the nuclear and magnetic contributions to the coherent scattering add for one of the two neutron spin states and subtract and cancel for the other when the atomic magnetic moments are fully aligned by an external magnetic field. Of those investigated to date, the consensus view is that the Heusler alloy crystal  $\text{Cu}_2\text{MnAl}$  is the best choice in terms of both reflectivity and polarizing efficiency. Detailed studies - such as those made, for example, by A. Freund et al,<sup>45</sup> have shown (i) that well annealed  $\text{Cu}_2\text{MnAl}$  crystals have (111) Bragg reflecting efficiencies that can approach those expected for ideally imperfect crystals, (ii) that the polarization of the reflected neutrons is in excess of 95% in crystals in which the Mn moments are fully aligned in an external field produced by permanent magnets, and (iii) that there is no significant loss of polarization when individual crystal plates are mounted so as to form a cylindrically-curved, vertically-focusing array.

We are aware that  $\text{Cu}_2\text{MnAl}$  crystals, like all polarizing crystals, are not without problems. One is that the procurement of crystals of good quality has been difficult in the past. We have been advised, however, that they can now be obtained from the ILL. A second is that the nuclear and magnetic contributions to the (222) Bragg reflection are not well-matched and second order contamination of the reflected beam can significantly reduce the polarizing efficiency. Fortunately this is ruled out as a potential problem for HYSPEC because the upstream choppers will deliver a higher-order-free, monochromatic beam to the crystal. And third, there is the issue of parasitic Bragg reflections which are known to have a non-negligible impact on both the polarizing efficiency and reflectivity and are likely to impair performance at certain neutron energies. The time-honored way to side-step this difficulty is simply to chose a crystal orientation that gives optimal performance at the energy at which the spectrometer will most often be used, in this case 15 meV, and incorporate messages into the operating software that warn experimenters about operating at those incident neutron energies where the polarizing efficiency and/or reflectivity is significantly affected by parasitic reflections. Since this will somewhat limit experimental flexibility, it is our intention to explore the feasibility of fabricating the individual plates in the vertical focusing array from stacks of 0.5 mm thick wafers cut from  $\text{Cu}_2\text{MnAl}$  single crystals. There are two potential advantages of this so-called “composite crystal” approach. One is that composite wafer stacks are not as spatially

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<sup>45</sup> A. Freund, et al, *Physica* 120B, 86 (1983)

coherent as monolithic crystals; this reduces parasitic reflections. The other is that introducing mosaic into the wafers by single-axis deformation before they are bonded together creates a highly anisotropic mosaic that improves the reflectivity without impacting the vertical focusing.

### 3.4.2 The Polarization Analyzers

Signal and background are typically of comparable intensity in polarization analysis measurements. Translated into practical terms, this means that definitive determination of the signal polarization will only be possible if both the polarizer and polarization analyzer have polarizing efficiencies in the 0.80–0.95 range. Heusler alloy polarizer crystals, which produce polarizations on the order of 0.90–0.95, easily meet this standard over the neutron energy range in which HYSPEC will operate. Because they are of comparable efficiency and are both well-tested and maintenance-free, our choice for analysis of the polarization of the scattered neutron beam is the supermirror-bender polarization analyzer. Reduced to essentials, this type of analyzer is nothing more than a short, curved multi-channel guide with magnetically-aligned, polarization-selective Fe-Si supermirror films on the channel walls. Because the angles of total reflection of the + and – spin states differ by more than a factor of three in such films, neutrons of one spin state tend to follow the curved channels while those of the other continue in their original direction. The incident beam is thus divided into divergent beams of opposite polarization. When the beam is well-collimated and the bender optimally curved and tilted, polarization analyzing efficiencies in the 0.80-0.95 range are easily achieved. Moreover, at sufficient analyzer-to-detector distances the two beams become spatially separated and both polarizations can be observed at the same time.<sup>46</sup>

To make the most effective use of the extended angular acceptance of the HYSPEC detector array, an equivalent array of bender analyzers would need to be installed, each directly downstream of a 20 minute angular acceptance collimator. Like all such analyzers presently in use, we envision that the bender channels would be formed by single crystal Si wafers with surface coatings of Fe-Si supermirror film. For HYSPEC the wafers would be 0.25 mm thick, 5 cm long and 14 cm high. To perform optimally at 15 meV, they would be horizontally bent to a radius of about 5 meters. Packed in groups of 80 into 3 cm exterior width thin-walled aluminum alloy containers, the wafer packs would form 2 cm wide, 80 channel benders. Room temperature single crystal Si, it should be noted, is sufficiently transparent to neutrons in the energy range of interest that scattering and absorption losses would not exceed 10 percent. Permanent magnets would be used to align the Fe moments in the Fe-Si films. Assuming the closest possible packing of the containers along an arc 55 cm from the sample axis, 19 such bender analyzers could be positioned within the (60 degree horizontal and 15 degree vertical) solid angle subtended by the detector array.

From the Monte Carlo (MC) simulation shown in Figure 3.3, it is evident that the spatial profiles of the two oppositely polarized beams would be completely separated at the detector bank 4.5 meters from the sample axis. It is also evident in the figure that the undeflected beam will spread over two (2.5 cm diameter) detectors and the oppositely polarized (somewhat wider) beam following the curved channels will fall on the adjacent

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<sup>46</sup> S.H. Lee and C.F. Majkrzak, *J. Neutron Res.* 7, 131 (1999)

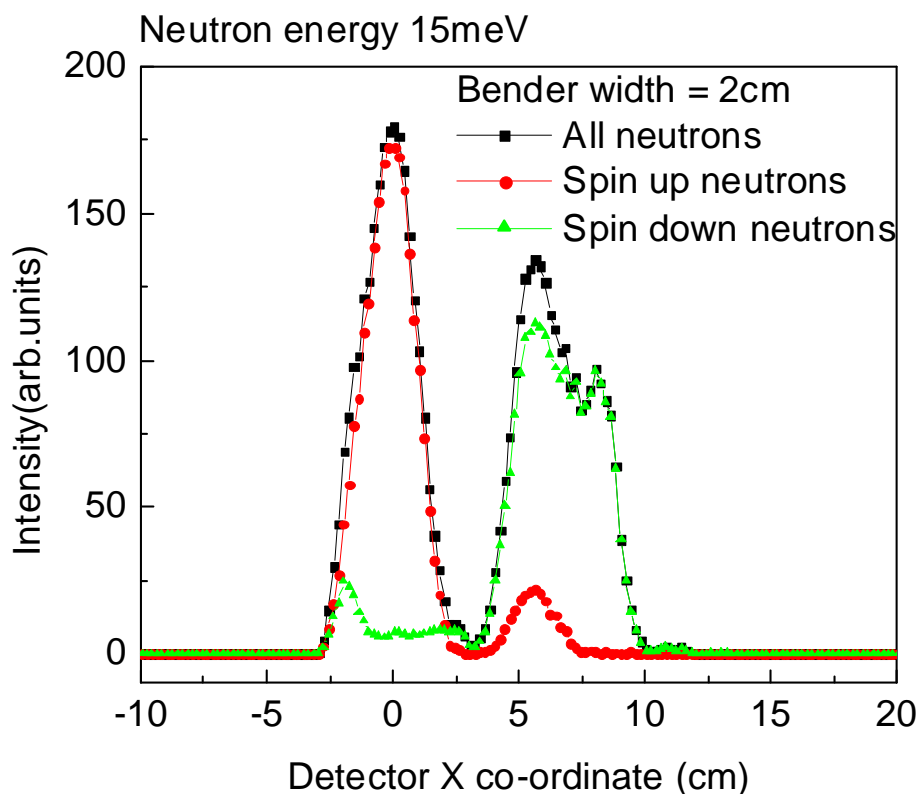


Figure 3.3. Spatial distribution of two neutron polarizations on the detector as created by a single supermirror-bender

three detectors. Considering that each bender analyzer unit would be centered on a group of 10 detectors, 50 percent of the detector array would be actively collecting data in this arrangement (which is very nearly optimum from the standpoint of maintaining adequate spatial separation of the beams from adjacent analyzers). Note that although each of the 19 analyzers is limited to a specific scattering angle, rotation of the detector bank around the sample axis will make it possible to cover - sequentially - the full scattered neutron angular range. No more than ten rotational steps of the detector would be needed to monitor both the flipped and unflipped spin intensities over the full 60 degree angular range covered by the detector array. It is also clear from the Figure 3.3 that the flipping ratio measured in some detectors is higher than that in the others (in which the peak of the “wrong” polarization occurs). Therefore, if the signal is sufficiently strong, it is possible to enhance the polarization sensitivity by restricting the counting to the detectors with the highest flipping ratios. This is equivalent to tightening the beam collimation after the bender-polarizer, but could be done by the experiment analysis software without repeating the actual measurement. Such flexibility is another attractive feature of the supermirror-bender polarization analysis scheme proposed for HYSPEC.

Figure 3.4 shows a MC simulation of bender analyzer performance over a range of energies on either side of 15 meV. From this it is evident that benders designed for optimum polarizing efficiency at 15 meV will operate with little loss of efficiency over

an energy range extending from roughly 8 to 18 meV. A second set of essentially identical bender analyzers configured for optimum performance at 5 meV would cover the energy range from about 3 to 8 meV with about the same efficiency, making it possible to span the entire scattered neutron range from 3 to 18 meV.

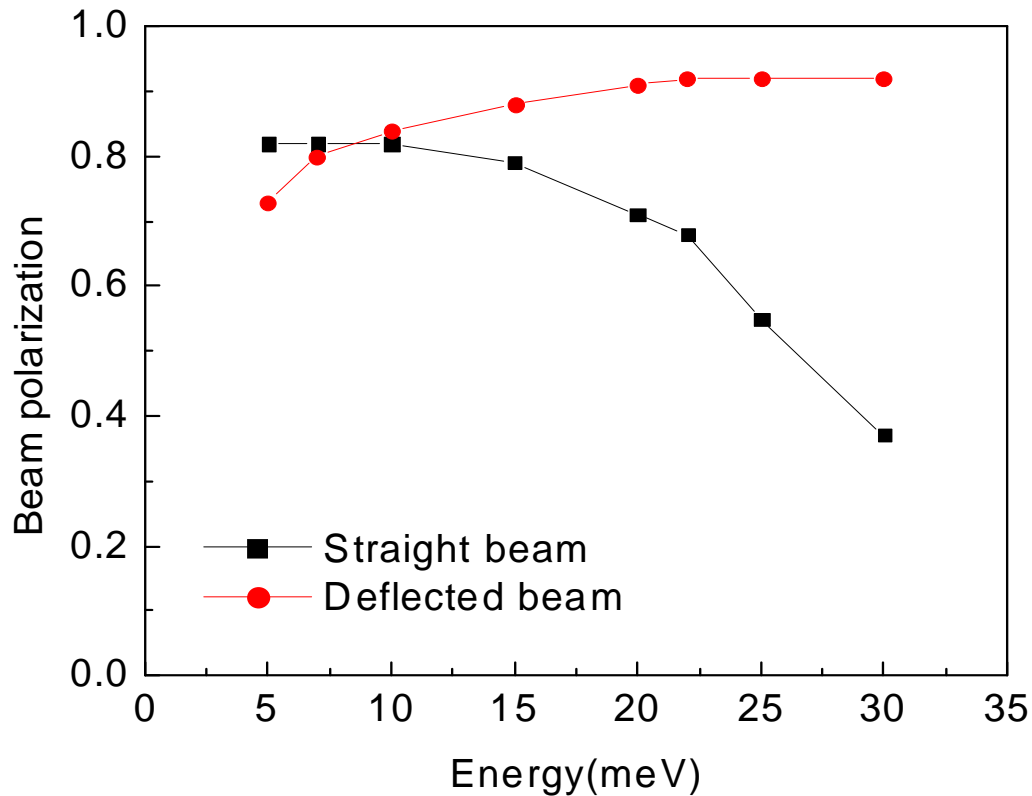
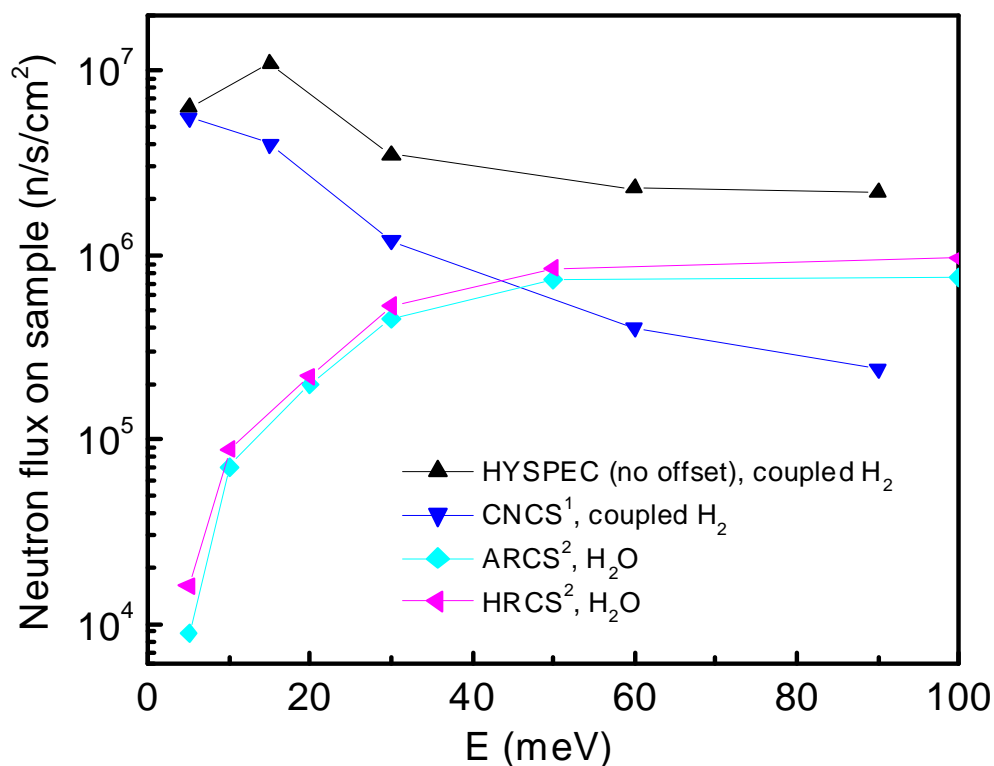


Figure 3.4. Average beam polarization in each of the two beams

Probably the most attractive feature of using bender analyzers in a time-of-flight energy analyzing system like HYSPEC's is the capability of monitoring *both* scattered neutron spin states simultaneously over a relatively broad scattered neutron energy range. But there are other attractions as well: bender analyzers are extremely stable and, as noted above, once built require little or no attention and are completely maintenance free.

### 3.5 Performance

Of the many special features of the instrument, the most important from the viewpoint of efficient use of source neutrons is the utilization of the superior focusing properties of curved crystals to concentrate the monochromatic flux on sample. To quantify the advantage of the HYSPEC concept in this respect, a number of MCSTAS, Monte-Carlo-based, flux-on-sample simulations were made to compare HYSPEC's flux-on-sample with that of other proposed SNS inelastic instruments. As is evident in Figure 3.5, despite the finite reflectivity of the PG crystal, its superior focusing properties concentrate the monochromatic flux more effectively than converging guides over the greatest part of the energy range in which HYSPEC will operate. For the moderate resolution, single crystal sample studies for which it is planned, the HYSPEC approach is markedly superior.



<sup>1</sup>CNCS model based on "Optimization...", J.V. Pearce et al.

<sup>2</sup>G. Granroth, Private communication

Figure 3.5. Calculated flux on sample for HYSPEC and other inelastic spectrometers planned for the SNS

### 3.6 Moderator Choice

Monte Carlo simulations have also shown that to perform optimally over the incident neutron energy range of interest (5-90 meV), a spectrometer of this type needs to be located on a beamline served by a coupled, 20 K, supercritical H<sub>2</sub> 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. Extending the instrument to an outside building would lead to a detrimental mismatch between the monochromating and analyzing resolutions and a nearly two-fold reduction of monochromatic flux at the sample position.

### 3.7 Additional Advantages of the HYSPEC Concept

Apart from the features described above, HYSPEC has many other attractive properties:

- Incident neutron energy selection and analysis of scattered neutron energies would be primarily by time-of-flight; thus full advantage is taken of the pulsed beam.
- Only two components – the counter-rotating chopper pair and the Fermi chopper –

would operate at high rotation speeds. Both would be of conventional design and would operate well within the limits imposed by the tensile strengths of the available materials.

- Moving the sample out of the direct beam and placing shielding between it and the detectors is expected to reduce beam-related background to a minimum.
- Near-forward sample scattering will be accessible to investigation.
- Depending on the type of measurement, the spectrometer operation could be optimized for either a wide angular acceptance or a selected Q-range.
- Apart from its focusing properties, the crystal also has the important effect of substantially reducing the (source produced) spectral asymmetry of the beam incident on the sample: the energy resolution function will be more symmetrical than on other instruments on coupled moderators.
- A relatively wide primary beam (4 cm) will be available thus making it possible to fully illuminate large as well as small samples.
- A broad and continuous range of incident neutron energies ( $5 \leq E_i \leq 90$  meV) will be accessible without order contamination.
- Energy resolution can be incrementally varied simply by changing the rotation rate of the counter-rotating and /or Fermi choppers.
- By changing the collimation of the incident monochromatic beam or the angular acceptance at the analyzer (or both) the longitudinal Q-resolution can easily be varied.
- Various kinds of monochromating crystals with a variety of focussing options could be employed such as, for example, two-dimensional focussing, asymmetrically-cut, perfect crystal focussing, etc.

### **3.8 Future Considerations**

Yet to be addressed in detail are two design issues. The first and most important relates to keeping the background to a minimum: a choice will have to be made between a curved guide with a beam stop inside the monochromator drum shield and a straight guide with a “get-lost” pipe with the beam stop a considerable distance from the data collecting area. The second issue is purely mechanical: the large (and heavy) analyzer of the spectrometer will have to be rigidly coupled to the large (and heavy) monochromator drum shield and move with it when the incident energy is changed. Additionally, the detector array will have to rotate in a precise and reproducible fashion about the sample axis. This, however, does not seem to pose any conceptual difficulty, as similar task is successfully accomplished in the design of several existing modern neutron spectrometers, such as FOCUS at Swiss Spallation Neutron Source SINQ, or a Spin-Echo machine recently commissioned at NIST Center for Neutron Research. There is also a location constraint: because the proposed secondary flight-path is sufficiently long (nominally 4.5 m), and in addition the sample axis is offset from the primary beam (1.8 m), the combined drum shield, analyzer and associated analyzer shielding will require an ample amount of space on the experimental floor and limit the choice of beam lines.

## 4. INSTRUMENT DEVELOPMENT TEAM

### 4.1 Membership and composition

The HYSPEC Instrument Development Team was formed following the Workshop on the Hybrid Spectrometer for the SNS held at BNL in October of 2001. Most of the IDT members participated in the workshop and have subsequently contributed to developing the HYSPEC science case, as well as to the technical issues, presented in this proposal. The IDT membership is open to qualified applicants upon a 2/3 majority vote of the Executive Committee.

The members of the IDT come from a variety of national and international universities and laboratories and are listed below. All have a common interest in the investigation of low energy, atomic-scale dynamical properties of crystalline solids. The IDT includes many senior members of the condensed matter community with well-established scientific credentials such as Tranquada, Lander, Shirane, Rhyne, etc. who expect to use HYSPEC to continue their research programs. The IDT also includes younger faculty members such as Lee, Greven, Kiryukin, Hirota who are still in the process of building their scientific programs and intend to use HYSPEC as one of their main research tools. Other members of the IDT have particular areas of expertise, which are vital to the project. For example, Majkrzak and Regnault are leading experts in polarized neutron beams; the Ames group (Stassis) has extensive experience in building large mechanical structures; and LANL (Daemen) is a leader in Monte Carlo simulations and has extensive experience in software development.

### 4.2 Organization and mission

The efforts of the Instrument Development Team are coordinated by the Executive Committee, which is headed by the Principal Investigators, S. Shapiro and I. Zaliznyak. It is expected that the membership in the Executive Committee will evolve as the project progresses. As is illustrated in the schematic organizational structure presented in Fig.5.1, the PI's and the Executive Committee closely interact with the SNS Instrument Systems Group and report to the DOE BES. SNS Instrument Scientist, D. Abernathy, currently serves as a liaison between the IDT Executive Committee and the SNS Instrument Systems Group. Based upon its expertise, the IDT provides input to the instrument design, engineering, construction and scientific program through the work of the various Topical Advisory Teams (TAT) with experience in polarized beams, detector technology, software, etc. These TAT's are coordinated by the Executive Committee. The IDT's ultimate mission is to ensure that the world's best state of the art instrument is built and commissioned at the SNS and will produce world class science.

#### Executive Committee:

<u>S. M. Shapiro</u> , co-PI	BNL
<u>I. Zaliznyak</u> , co-PI	BNL
J. Tranquada	BNL
L. Passell	BNL
C. Stassis	Ames Lab/Iowa St. University
D. Abernathy	SNS



**IDT Members with their institutional affiliations:**

J. Gardner	BNL
V. J. Ghosh	BNL
G. Shirane	BNL
G. Xu	BNL
L. Daemon	Los Alamos
M. Greven	Stanford University
B. Gaulin	McMaster University
K. Hirota	ISSP
V. Kiryukhin	Rutgers University
G. Lander	EITU
Y. Lee	MIT
C. Majkrzak	NIST
S. Nagler	ORNL
R. Osborn	Argonne
L. P. Regnault	CEN-Grenoble
J. Rhyne	Missouri University
A. Zheludev	ORNL

**5. PROJECT MANAGEMENT PLAN**

A schematic of the proposed project organizational structure is presented in Figure 5.1. We propose that the project is directed by the HYSPEC Executive Committee headed by the Principal Investigators in close coordination with the SNS Instrument Systems Group. The PI's, on behalf of the IDT Executive Committee, will interact closely with the SNS Experimental Facilities Division and report to the DOE BES. They will also interact with the SNS to establish the framework for the practical implementation of the project which will be documented in the form of the HYSPEC Top Level Specifications (TLS). The draft version of the TLS is attached in Appendix C. The final working version will be negotiated, agreed, and co-signed by the SNS and the HYSPEC IDT management.

In the proposed plan the Center for Neutron Science (CNS) at Brookhaven National Laboratory continues to play a central role in the HYSPEC project. This is natural in view of the role it has played in designing and developing the spectrometer and also benefits BNL's Neutron Scattering Group. We believe that such a role also benefits the national neutron effort by diversifying the DOE's neutron instrumentation capabilities. At the same time we understand that a final decision on the structure of the Management Plan remains to be made.

In our plan the HYSPEC Instrument Scientist (FTE) and a Project Engineer (FTE) would be subcontracted to the BNL Center for Neutron Science in a manner consistent with the DOE BES policy concerning the SNS Instrument Construction Projects. They will be responsible for the project oversight and day-to-day operations as a project manager and an assistant project manager, respectively. They will work with the component teams of the SNS Instrument Systems Group and under the supervision of the IDT Executive Committee, and will report to the HYSPEC PI's. An additional workforce at BNL in the form of the postdoctoral research associates and/or the part-time assistants will be funded as necessary for the instrument design and engineering studies, software development,

scientific program development, etc. Engineering and technical resources of the SNS Instrument Team at Argonne National Laboratory and SNS/ORNL will be subcontracted as needed for the design, engineering, fabrication and installation of the instrument components and consistent with the DOE policy.

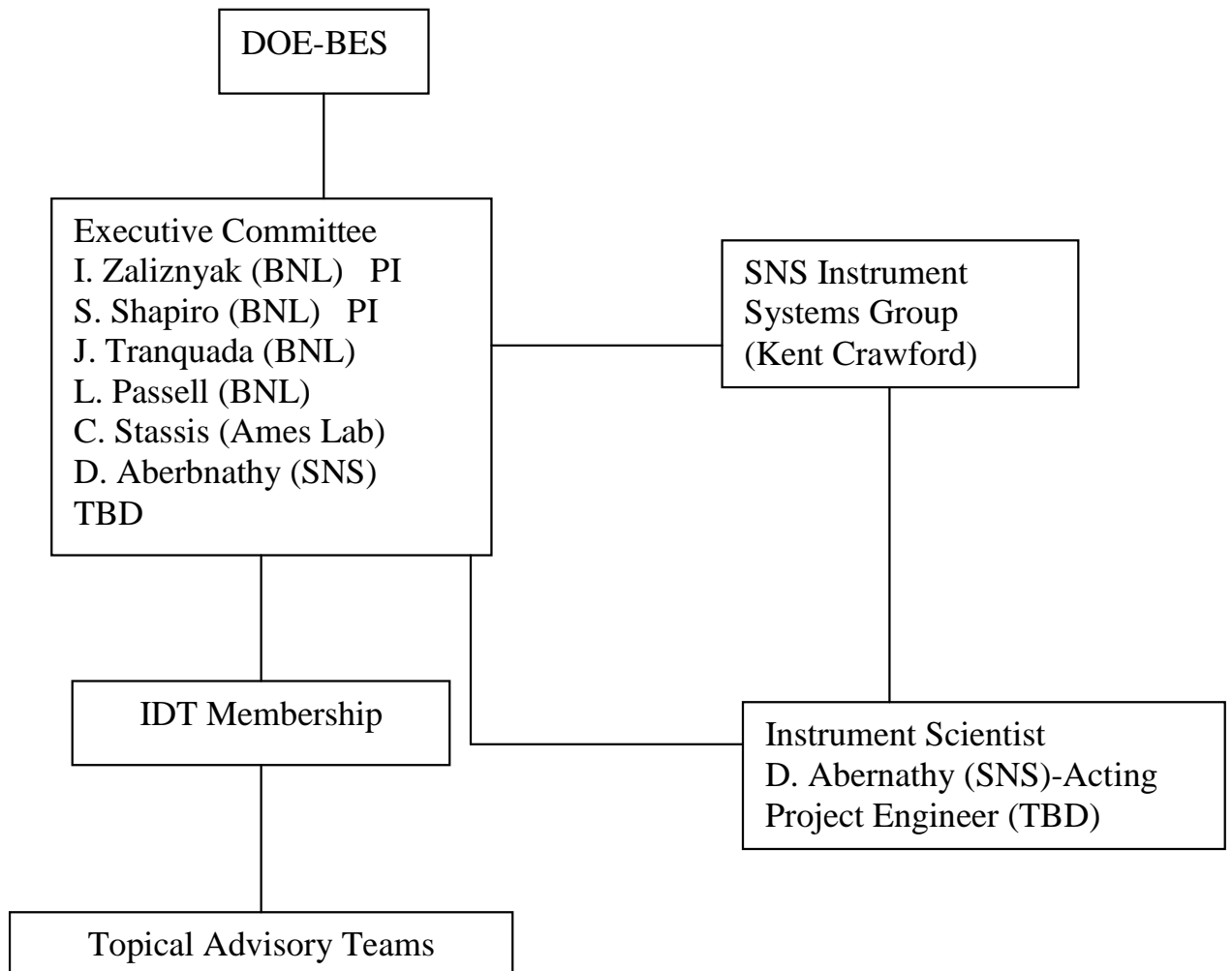


Figure 5.1 Organizational Structure

The project management responsibilities will include (i) preparing the detailed design specifications of the instrument systems and components following the IDT guidance and in compliance with the TLS; (ii) preparing the detailed budget estimates, asking for bids, and negotiating with the subcontractors for the outsourced components; (iii) working with the SNS to oversee the in-house fabricated components subcontracted to the SNS Instrument Systems Group and closely coordinate the purchase orders for the externally outsourced components to maximize the economy of scale wherever possible; (iv) overseeing the installation and integration of the instrument systems; (v) directing the software development; (v) participating in the instrument commissioning and user scientific program development. The Instrument Scientist will also interact with the DOE

BES and the SNS to report on significant developments and issues, and to fulfill the general reporting and other requirements appropriate for a construction project.

## 6. ESTIMATED BUDGET AND TIME SCALE

The HYSPEC cost summary is shown in Table II, a detailed budget estimate and funding profile are presented in Appendix D. The budget was estimated after consultations with the SNS Instrument Systems Team and using the SEQUOIA<sup>47</sup> and ARCS<sup>48</sup> proposed budgets as guidelines for items which would be common to HYSPEC, such as shielding, detectors, choppers, etc. There has been minimal engineering input for HYSPEC so far, which will be vital to firm up these costs. Therefore, this budget is preliminary and will be modified after more detailed engineering and design studies are undertaken. To this end, we are initially asking for \$130K in FY03 and \$400K in FY04 to hire a project engineer and a project scientist who would direct the essential engineering that is needed for a Conceptual Design Report (CD1).

The HYSPEC estimated cost is \$15,750K in FY03 dollars, including burden and contingency. Escalated to as spent dollars, the cost would be \$18,239K at end of project. This covers construction of an optimized instrument located within the experimental hall. However there is concern expressed by the SNS Instrument Systems Team leader that the siting of HYSPEC will interfere with neighboring beam lines, which have not yet been allocated. One possibility is to locate HYSPEC in a separate building outside of the experimental hall. This will result in additional costs due to the building and the extra guides and shielding that will be needed. A rough estimate is \$3M for the building and an additional \$1.25M for the guides and shielding. The IDT is concerned, however, that extending the instrument will severely compromise its performance: at a fixed analyzer resolution an increase in the primary flight-path results in roughly proportional decrease in the flux-on-sample; calculations are underway to establish the performance of such an extended instrument more precisely (see also Appendix C).

The profile given in Table II is five years from the onset of funding based upon estimates for ARCS and SEQUOIA. However, because of the limited engineering studies that have been performed it is likely that the funding profile would be extended to 6 or 7 years to allow for the initial engineering studies. It will also be necessary to discuss with SNS the practical timing of spectrometer installation.

The budget includes a substantial funding, 200k\$ per year, for scientific program development. This is necessary not only to ensure that the HYSPEC IDT remains at the forefront of neutron research but also that new opportunities provided by the SNS and the HYSPEC spectrometer are developed and utilized to the fullest extent. It is also needed to ensure that the young scientists who will form the core of the future user community have opportunities for appropriate scientific development. The scientific program will be developed under the supervision of the IDT members. This funding will be used to hire postdoctoral fellows who will participate in spectrometer development and will be

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<sup>47</sup> "HRCS Instrument Summary for IDT", G. Ganroth, July 8, 2002

<sup>48</sup> "Possibilities for High-Energy Chopper Spectrometers at the SNS", written for the ARCS Instrument Development Team meeting 4/30/01 in Pasadena, CA by Doug Abernathy, 4/23/01

involved in research using existing chopper spectrometers around the world, to pay for travel and sample preparation for the experiments, etc.

Finally, there have been recent communications between the co-PI (Shapiro) and the French IDT member, L.P. Regnault, who has stated that the French Atomic Energy Commission (CEA) is considering a possibility of participating in HYSPEC project by providing some funds for it. Obviously, we are vigorously pursuing this.

**Table II. HYSPEC Estimated Cost and Funding Profile**

ITEM	FY03 Cost Estimate	At Year Funding Required						Total
		FY03	FY04	FY05	FY06	FY07	FY08	
<b>Technical Construction</b>								
Primary Flight Path	3,300	0	0	1,603	1,930	0	0	3,533
Monochromator Section	2,560	0	0	380	2,385	0	0	2,765
Sample Stage	350	0	0	158	108	111	0	378
Detector System	3,440	0	0	717	2,993	0	0	3,710
Data Collection System	400	0	256	0	11	11	148	426
Installation Labor	1,400	0	0	0	0	445	1,140	1,585
Technical Construction Total	11,450	0	256	2,858	7,427	567	1,288	12,398
<b>Project Management &amp; Engineering</b>								
Project Management	800	0	164	169	173	178	182	867
Engineering & Design	2,500	405	513	522	537	384	296	2,657
Proj. Mgt & Engrg. Total	3,300	380	615	628	645	940	1,551	4,758
<b>Project TEC</b>	<b>14,750</b>	<b>380</b>	<b>871</b>	<b>3,486</b>	<b>8,072</b>	<b>1,507</b>	<b>2,839</b>	<b>17,156</b>
<b>Other Costs</b>	<b>1,000</b>	<b>0</b>	<b>205</b>	<b>211</b>	<b>217</b>	<b>222</b>	<b>228</b>	<b>1,083</b>
<b>Total Project Cost (TPC)</b>	<b>15,750</b>							<b>18,239</b>

## Appendix A. CV of the HYSPEC IDT Members

### Stephen M. Shapiro

**Name and Date of Birth:** Stephen M. Shapiro  
June 21, 1941

**Address** Brookhaven National Laboratory  
Department of Physics  
Upton, NY 11973  
631-344-3822  
[shapiro@bnl.gov](mailto:shapiro@bnl.gov)

**Education:** 1969, Ph.D. Johns Hopkins University  
Thesis: Light Scattering Study of Alpha-Beta Transition in Quartz; H. Z. Cummins, advisor  
1963, B.S., Union College

**Employment** 2001-present, Director of Center for Neutron Science  
2000-present, Senior Physicist  
1994-2000: Head of Solid State Physics  
1994: Visiting Professor, University of Grenoble  
1986-1987: Distinguished Visiting Scientist, Laboratoire Léon Brillouin, Saclay, France  
1983: Yamada Fellowship, University of Osaka, Japan  
1975-2000: Physicist (with tenure, 1984), Brookhaven  
1972-1975: Associate Physicist, Brookhaven  
1971-1972: Research Associate, Brookhaven  
1969-1972: Postdoctoral Fellow, University of Paris

**Professional Societies:** American Physical Society  
Materials Research Society (MRS)  
Neutron Scattering Society of America (NSSA)

**Committees** Program Advisor Committees for IPNS and LANSCE  
Chaired Program Review Committee of AECL, Chalk River, Canada  
Past Treasurer, Neutron Scattering Society of America (NSSA)  
US-Japan Steering Committee Member  
Divisional Associate Editor for Physical Review Letters  
Member of Scientific Advisory Committee of CEA, France  
Chair, Review Committee for CEA-Grenoble, Neutron Program

**Awards and Honors:** Fellow of the American Physical Society 1986  
DOE Award for Outstanding Scientific Accomplishment in 1988 for work on Premartensitic Behavior in metallic alloys

**Publications:** 1. *Optical Response of High-Dielectric-Constant Perovskite-Related Oxide*, C. C. Homes, To. Vogt, S. M. Shapiro, A. P. Ramirez, *Science* **293**, 673 (2001).  
2. *Field-Induced Three- and Two-Dimensional Freezing in a Quantum Spin Liquid*, Y. Chen, Z. Honda, A. Zheludev, C. Broholm, K. Katusmata, and S. M. Shapiro, *Phys. Rev. Lett.* **86**, 1618 (2001).

3. *Electron Diffraction Studies of Phonons and Static Disorder in SrTiO<sub>3</sub>*, R. Wang, Y. Zhu, and S. M. Shapiro, Phys. Rev. B 621, 8814 (2000).
4. *Neutron Scattering Studies of Pre-transitional Effects in Solid-Solid Phase Transformations* S. M. Shapiro, Proceedings of PTM-99, Kyoto, May 1999 (Japan Institute of Metals Proceedings, **12**, 799 (2000))
5. *Structural Defects and the Origin of the Second Length Scale in SrTiO<sub>3</sub>*, R. Wang, Y. Zhu, and S. M. Shapiro, Physical Review Letters **80**, 2370 (1998)

## Igor A. Zaliznyak

- Date of Birth:** 05/01/1965
- Professional Address:** Physics Department, Brookhaven National Laboratory (BNL), Upton, NY 11973-5000, USA.  
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Email: [zaliznyak@bnl.gov](mailto:zaliznyak@bnl.gov); [igor@neutrons.phy.bnl.gov](mailto:igor@neutrons.phy.bnl.gov)
- Education:** Ph. D. in Physics (1993), P. Kapitza Institute for Physical Problems, Moscow, Russia. Thesis title: *Experimental study of the magnetostatic and resonance properties of quasi-one-dimensional antiferromagnets*. Thesis supervisors: L. A. Prozorova and L.-P. Regnault
- Employment:** Associate Physicist, 2001 – present; Assistant Physicist, 1999-2001, Neutron Scattering Group, Brookhaven National Laboratory, Upton, NY
- Postdoctoral Research Fellow, 1996-1999, Department of Physics and Astronomy, Johns Hopkins University, Baltimore, MD
- Visiting researcher, 11/1995-01/1996; 08/1994-09/1995, Laboratoire de Magnetisme et Diffraction des Neutrons, SPSMS/DRFMC, CEN-Grenoble, France
- Scientist, 1995-; Junior Scientist, 1993-1995, P. Kapitza Institute for Physical Problems, Moscow, Russia.
- Visiting (graduate) researcher, 12/1991-06/1993, Laboratoire de Magnetisme et Diffraction des Neutrons, SPSMS/DRFMC, CEN-Grenoble, France
- Professional Societies:** Member, American Physical Society (APS), Neutron Scattering Society of America (NSSA)
- Committees:** Member, SNS-HIFR User Group, Oak Ridge National Laboratory, TN; Member, Solid State Future Planning Committee, BNL
- Awards and Honors:** Presidential fellowship for outstanding young researcher, Moscow, Russia, 1993-1995; "Red" diploma of excellence, Moscow Institute of Physics and Technology, Russia, 1988
- Recent Publications:**
- A. Zaliznyak, C. Broholm, M. Kibune, H. Takagi, "Spin Freezing In The Cuprate  $S=1/2$  Antiferromagnetic Chain Compound  $\text{SrCuO}_2$ ", cond-mat/9812440 (1998); Phys. Rev. Lett. **83**, 5370 (1999).
  - I. A. Zaliznyak, J. P. Hill, J. M. Tranquada, R. Erwin, Y. Moritomo "Independent freezing of charge and spin dynamics in  $\text{La}_{1.5}\text{Sr}_{0.5}\text{CoO}_4$ ", cond-mat/0006115, Phys. Rev. Lett. **85**, 4353 (2000).
  - I. A. Zaliznyak, S.-H. Lee, S. V. Petrov, "Continuum in the spin excitation spectrum of a Haldane chain, observed by neutron scattering in  $\text{CsNiCl}_3$ " cond-mat/0010049; Phys. Rev. Lett. **87**, 017202 (2001).
  - M. B. Stone, I. Zaliznyak, D. H. Reich and C. Broholm, "Frustration-Induced Two Dimensional Quantum Disordered Phase in Piperazinium Hexachlorodocuprate", cond-mat/0104150; Phys. Rev. B

- 64**, 144405 (2001).
- I. A. Zaliznyak, J. M. Tranquada, R. Erwin, Y. Moritomo, "Spin-entropy driven melting of the charge order in  $\text{La}_{1.5}\text{Sr}_{0.5}\text{CoO}_4$ ", cond-mat/0105404; Phys. Rev. B **64**, 195117 (2001).
  - I. A. Zaliznyak, "Continuum Spin Excitations in S=1 one-dimensional antiferromagnet", cond-mat/0109065; J. Appl. Phys. 91 812210MMM (2002).



## JOHN M. TRANQUADA

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**Educational Background:** B.A., cum laude, in Physics, Pomona College, 1977  
Ph.D. in Physics, University of Washington, 1983  
Thesis: "X-ray Absorption Studies of Solids at High Pressure";  
Advisor: Robert Ingalls

### Professional Experience:

*1983-1986:* Postdoctoral Research Associate, North Carolina State University and Brookhaven National Laboratory  
*1986-1988:* Assistant Physicist, Brookhaven National Laboratory  
*1988-1990:* Associate Physicist, Brookhaven National Laboratory  
*1990-2000:* Physicist, Brookhaven National Laboratory (with tenure since 1992)  
*1998-present:* Leader of Neutron Scattering Group, Brookhaven National Laboratory  
*2000-present:* Senior Physicist, Brookhaven National Laboratory

### Professional Affiliations:

Fellow, American Physical Society  
Member, American Association for the Advancement of Science

### Other Professional Activities:

Member of the Steering Committee for the US-Japan Cooperative Research Program on Neutron Scattering, 1999-  
BESAC Subpanel on Neutron Scattering, 2000  
BESAC Subpanel Review of IPNS and MLNSC, 2000  
SNS-HFIR User Group (SHUG) Executive committee, 2000-present Vice-Chair, 2001; Chair, 2002  
Divisional Associate Editor, Physical Review Letters, 2001-present  
Lehman Review Committee for the Spallation Neutron Source, 2001-present  
Member of the Program Advisory Committee for NCNR (NIST), 2001-present  
Member of the Proposal Review Committee for HFIR (ORNL), 2002

### Honors and Awards:

DOE Award for Outstanding Scientific Accomplishment in Solid State Physics, 1988  
Fellow of the American Physical Society, 1997  
BNL R&D Award, 1997

### Recent Publications

1. V. J. Emery, S. A. Kivelson, and J. M. Tranquada, "Stripe Phases in High Temperature Superconductors," *Proc. Natl. Acad. Sci. U.S.A.* **96**, 8814-7 (1999).

2. N. Ichikawa, S. Uchida, J. M. Tranquada, T. Niemi, P. M. Gehring, S.-H. Lee, and J. R. Schneider, "Local Magnetic Order vs. Superconductivity in a Layered Cuprate," *Phys. Rev. Lett.* **85**, 1738-41 (2000).
3. I. A. Zaliznyak, J. P. Hill, J. M. Tranquada, R. Erwin, and Y. Moritomo, "Independent freezing of charge and spin dynamics in  $\text{La}_{1.5}\text{Sr}_{0.5}\text{CoO}_4$ ," *Phys. Rev. Lett.* **85**, 4353 (2000).
4. J. M. Tranquada, K. Nakajima, M. Braden, L. Pintschovius, and R. J. McQueeney, "Bond-Stretching-Phonon Anomalies in Stripe-Ordered  $\text{La}_{1.69}\text{Sr}_{0.31}\text{NiO}_4$ ," *Phys. Rev. Lett.* **88**, 075505 (2002).
5. S.-H. Lee, J. M. Tranquada, K. Yamada, D. J. Buttrey, Q. Li, and S.-W. Cheong, "Freezing of a Stripe Liquid," *Phys. Rev. Lett.* **88**, 126401 (2002).

## Jason Stewart Gardner

### Personal Data

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Nationality: British

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### University Qualifications

**(1988-91)**

B. Sc. (Physics), University of Warwick,  
Coventry, England.

**(1991-92)**

MSc. (Physics), Keele University,  
Staffordshire, England.  
For a course entitled "Optical Data Recording"

**(1992-96)**

Ph.D. (Physics), University of Warwick,  
Coventry, England

### Thesis Title:

"Neutron Scattering,  $\mu$ SR and Magnetic Studies of Compounds Related to High Temperature Superconductors."

### Thesis Supervisor:

Professor Donald M<sup>c</sup>Kenzie Paul

### Professional Employment

#### ***(Nov 2002 – Present)***

I am currently an assistant physicist for the Brookhaven National Laboratory. I am part of the Brookhaven / National Institute of Standards and Technology (NIST) alliance to promote research, specifically neutron scattering, in the USA. My work will involve the study of prototypical magnets and structural materials using elastic and inelastic neutron scattering, as well as other tools that will help elucidate the properties being studied.

**(1999 – 2002):**

Research Associate, National Research Council, Chalk River Laboratories, Chalk River, CANADA.

**(1998 – 1999):**

Postdoctoral Fellow, Los Alamos National Laboratory, USA.  
Supervisors: Drs. D. Argyriou and R. H. Heffner

**(1996 – 1998):**

Research associate, Department of Physics and Astronomy, McMaster University, Canada.  
Supervisor: Prof. B. D. Gaulin

**(Summer 1990):**

Summer research assistant at the University of Oporto, Portugal. My work included measuring the thermopower and resistance of high $T_c$  superconductors. Supervisor: Prof. J. B. Sousa

**Awards/Grants**

**2002**

Three Researcher Exchange Awards between the NRC and the British Council \$6.5k  
NATO science Programme Collaborative Linkage Grant 10k EURO

**2001**

**Technology Investment Fund (TIF) with Dr. Calvin Hyatt**  
**- Design of Magnetic Shape Memory Alloys for 3 years**  
**\$250k/yr (3 yrs)**

Travel grant to Taiwan under the NRC's Eminent Researchers Program. \$5k  
Two Researcher Exchange Awards between the NRC and the British Council \$4.6k

**2000**

NSERC Major equipment Grant with M. Collins (McMaster University)  
9 Tesla, 300 mK superconducting magnet for neutron studies \$260k

**SELECTED PUBLICATIONS**

"Evidence for Quantum Dynamics in "Hot" Spin Ice"

G Ehlers, A L Cornelius, M Orendáč, M Kajňáková, T Fennell, S T Bramwell and **J. S. Gardner**  
Accepted to J. Phys. Cond. Matter (Nov, 2002).

"Pressure Induced Crystallization of a Spin Liquid"

I Mirebeau, I N Goncharenko, P Cadavez-Peres, S T Bramwell, M J P Gingras and **J S Gardner**  
NATURE **420**, 54 (2002).

"Magnetic structure of antiferromagnetic NdRhIn5"

S Chang, P G Pagliuso, W Bao, **J S Gardner**, I P Swainson, J L Sarrao, and H Nakotte  
Phys. Rev. B **66**, 132417 (2002).

Magnetization distribution in the Layered Colossal Magnetoresistance Manganite  $\text{La}_{1.2}\text{Sr}_{1.8}\text{Mn}_2\text{O}_7$  from Polarized Neutron Diffraction"

D.N. Argyriou, P.J. Brown, **J S Gardner** and R.H. Heffner  
Phys. Rev. B **65**, 214431 (2002).

"Neutron scattering studies of the cooperative paramagnet pyrochlore  $\text{Tb}_2\text{Ti}_2\text{O}_7$ "

**J S Gardner**, B D Gaulin, A J Berlinsky, P Waldron, S R Dunsiger, N P Raju and J E Greedan  
Phys. Rev. B **64**, 224416 (2001).

"Order in the Heisenberg pyrochlore: The magnetic structure of  $\text{Gd}_2\text{Ti}_2\text{O}_7$ "  
J D M Champion, A S Wills, T Fennell, S T Bramwell, **J S Gardner** and M A Green  
Phys. Rev. B **64**, 140407(R) (2001).

"Spin Correlations in  $\text{Ho}_2\text{Ti}_2\text{O}_7$ : a Dipolar Spin Ice System"  
S T Bramwell, M J Harris, B C Den Hertog, M J P Gingras, **J S Gardner**, D F McMorrow, A R Wildes,  
A Cornelius, J D M Champion, R G Melko and T Fennell  
Phys. Rev. Lett. **87**, 047205 (2001).

"Low Temperature Spin Dynamics of the Geometrically Frustrated Antiferromagnet  $\text{Gd}_3\text{Ga}_5\text{O}_{12}$ "  
S Dunsiger, **J S Gardner**, J Chakhalian, R Kiefl, R Movshovich W A MacFarlane, R I  
Miller, J E Sonier and B D Gaulin  
Phys. Rev. Lett., **85**, 3504 (2000).

"Magnetic and Thermodynamic Properties of the Collective Paramagnetic State in the Pyrochlore  
Antiferromagnet  $\text{Tb}_2\text{Ti}_2\text{O}_7$ "  
M J P Gingras, B C den Hertog, M Faucher, **J S Gardner**, S Dunsiger, L J  
Chang, B D Gaulin, N P Raju and J E Greedan  
Phys. Rev. B, **62**, 6496 (2000).

"Glassy Statics and Dynamics in the Chemically Ordered Pyrochlore Antiferromagnet  $\text{Y}_2\text{Mo}_2\text{O}_7$ "  
**J S Gardner**, B D Gaulin, S H Lee, C Broholm, N P Raju and J E Greedan  
Phys. Rev. Lett., **83**, 211 (1999).

## VINITA J. GHOSH

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**Education:** 1969 B.Sc. Physics University of Delhi, New Delhi, India  
1971 M.Sc. Physics University of Delhi, New Delhi, India  
1979 Ph.D. Physics University of Rochester, Rochester, NY  
Advisor: Robert S. Knox, Topic: Theory of hole transport in rare gas solids

**Employment History:** Physical Review and physical review Letters: 1980-1981  
Brookhaven National Laboratory: 1981-2000  
Consultant to Brookhaven National Laboratory: 2001-now

### **Selected Publications:**

V. J. Ghosh, M. McKeown, D. O. Welch, and K. G. Lynn. An *ab initio* Monte Carlo study of low energy positron and electron implantation in elemental metals and multilayers. Nucl. Instrum. Methods in Physics Research **B90**, 442-5 (1994).

V. J. Ghosh. Positron implantation profiles in elemental and multilayer systems. Appl. Surf. Sci. **85**, 187-95 (1995).

V. J. Ghosh and G. C. Aers. Positron stopping in elemental systems: Monte Carlo calculations and scaling. Phys. Rev. B **45**(1), 45-59 (1995).

K. A. Ritley, V. J. Ghosh, K. G. Lynn, M. Mckeown, and D. O. Welch. The SPRITE and POS-SPRITE user report: An extensible calculation of positron and electron implantation in solids, BNL-64884, Informal Report, (1997). This User Report is part of a package submitted to the DOE Science and Technology Software Center. It accompanies a collection of programs developed at BNL to calculate the trajectories of positrons and electrons in solids. These programs include the calculation of scattering cross-sections relating to positron and electron energy loss and thermalization in metals and small band-gap semiconductors.

Vinita J. Ghosh, Bent Nielsen, and Thomas Friessnegg. Identifying open-volume defects in doped and undoped perovskite-type  $\text{LaCoO}_3$ ,  $\text{PbTiO}_3$ , and  $\text{BaTiO}_3$ . Phys. Rev. **B61**, 207, (2000).

V.J. Ghosh, M. Alatalo, P. Asoka-Kumar, B. Nielsen, K.G. Lynn, A.C. Kruseman, and P.E. Mijnders, Calculation of the Doppler broadening of the electron-positron annihilation radiation in defect-free bulk materials. Phys. Rev. **B61**, 10092, (2000).

Vinita J. Ghosh, John Z. Larese, L.L. Daemen, and P.A. Seeger. Monte Carlo simulations of the HERMES spectrometer. (2000), (unpublished).

L.L. Daemen, V.J. Ghosh, L. Passell, and P.A. Seeger. A Proposed Q-Selective Time-of-Flight Spectrometer for Inelastic Neutron Scattering at the SNS, (2000) (unpublished).

## Martin Greven

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Stanford University  
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- Research Interests:** Neutron and x-ray scattering of strongly correlated electron systems. High-temperature superconductivity. Low-dimensional magnetism. Crystal growth and characterization. Quantum Monte Carlo simulations of model magnets.
- Education:** 1988: Vordiplom, Universität Heidelberg, Germany.
- 1988-89: Exchange Scholarship, University of Massachusetts, Amherst.
- 1989-95: Ph.D., Physics Department, Massachusetts Institute of Technology, with Prof. R.J. Birgeneau. Thesis title: "Neutron Scattering Study of Magnetism in Insulating and Superconducting Lamellar Copper Oxides."
- Employment:** 1995-97: Post-doc with Prof. R.J. Birgeneau, Massachusetts Institute of Technology.
- 1998-present: Assistant Professor, Department of Applied Physics and Stanford Synchrotron Radiation Laboratory, Stanford University.
- Professional Societies:** American Association for the Advancement of Science  
American Physical Society  
Neutron Scattering Society of America  
Materials Research Society
- Awards and Honors:** 1988-89: Exchange Scholarship, University of Massachusetts.  
1999-01: Alfred P. Sloan Fellow
- Selected Publications:** O.P. Vajk, P.K. Mang, M. Greven, P.M. Gehring, and J.W. Lynn, "Quantum impurities in the two-dimensional spin one-half Heisenberg antiferromagnet," *Science* 295, 1691 (2002).
- Y.J. Kim, A. Aharony, R. J. Birgeneau, F.C. Chou, O. Entin--Wohlman, R.W Erwin, M. Greven, A.B. Harris, M.A. Kastner, I.Y.

Korenblit, Y.S. Lee, and G. Shirane, "Ordering due to quantum fluctuations in  $\text{Sr}_2\text{Cu}_3\text{O}_4\text{Cl}_2$ ," Phys. Rev. Lett. 83, 852 (1999).

R.J. Birgeneau, M. Greven, M.A. Kastner, Y.S. Lee, B.O. Wells, Y. Endoh, K. Yamada, and G. Shirane, "Instantaneous spin correlations in  $\text{La}_2\text{CuO}_4$ ," Phys. Rev. B 59, 13788 (1999).

H. Kimura, K. Hirota, H. Matsushita, K. Yamada, Y. Endoh, S.-H. Lee, C.F. Majkrzak, R. Erwin, G. Shirane, M. Greven, Y.S. Lee, M.A. Kastner, and R. J. Birgeneau, Neutron scattering study of static antiferromagnetic correlations in  $\text{La}_{2-x}\text{Sr}_x\text{Cu}_{1-y}\text{Zn}_y\text{O}_4$ ," Phys. Rev. B 59, 6517 (1999).

K. Yamada, C.H. Lee, K. Kurahashi, J. Wada, S. Wakimoto, S. Ueki, H. Kimura, Y. Endoh, S. Hosoya, G. Shirane, R.J. Birgeneau, M. Greven, M.A. Kastner, and Y.J. Kim, "Doping dependence of the spatially modulated dynamical spin correlations and the superconducting transition temperature in  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ ," Phys. Rev. B 57, 6165 (1998).

M. Greven, R. J. Birgeneau, Y. Endoh, M. A. Kastner, B. Keimer, M. Matsuda, G. Shirane, and T. R. Thurston, "Spin correlations in the 2d Heisenberg antiferromagnet  $\text{Sr}_2\text{CuO}_2\text{Cl}_2$ : Neutron scattering, Monte Carlo simulation, and theory," Phys. Rev. Lett. 72, 1096 (1994).



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- Education:** Ph.D. (Physics), Nov 1997, Princeton University, Princeton, NJ
- M.S., Sep 1992, Moscow Institute of Physics and Technology,  
Moscow, Russia
- Ph.D. Thesis Title: Magnetism and Electron-Lattice Interaction:  
X-ray Scattering Study of Spin-Peierls and Colossal  
Magnetoresistance Systems
- Ph.D. Thesis Advisor: B. Keimer
- Employment:** Sep 1992-Aug 1997 Princeton University, Research Assistant  
Sep 1997-Aug 1999 MIT, Postdoctoral Research Assistant  
Sep 1999-present Rutgers University, Assistant Professor
- Professional Societies:** American Physical Society
- Committees:** 1. Program Committee, 46th Annual Conference on Magnetism and  
Magnetic Materials, July 2001.  
2. Proposal Study Group, Cooperative Grunts Program,  
U.S. Civilian Research and Development Foundation, May  
1996.
- Awards and Honors:** 2001 Alfred P. Sloan Foundation Award  
2001 NSF CAREER Grant Award
- Publications:**
1. T. Y. Koo, P. M. Gehring, G. Shirane, V. Kiryukhin, G. Lee, S-W. Cheong, "Anomalous transverse acoustic phonon broadening in the relaxor ferroelectric  $\text{Pb}(\text{Mg}_{1/3}\text{Nb}_{2/3})_{0.8}\text{O}_3$ ", Phys. Rev. B 65, 144113 (2002).
  2. V. Kiryukhin, Y.-J. Kim, F. C. Chou, K. J. Thomas, R. W. Erwin, Q. Huang, M. A. Kastner, R. J. Birgeneau, "Magnetic properties of the  $S=1/2$  quasi-one-dimensional magnet  $\text{CaCu}_2\text{O}_3$ ", Phys. Rev. B 63, 144418 (2001).
  3. P. G. Radaelli, Y. Horibe, M. J. Gutmann, H. Ishibashi, C. H. Chen, R. M. Ibers, Y. Koyama, Y.-S. Hor, V. Kiryukhin, and S-W. Cheong, "Formation of isomorphous  $\text{Ir}^{3+}$  and  $\text{Ir}^{4+}$  octamers and spin dimerisation in the spinel  $\text{CuIr}_2\text{S}_4$ ", Nature (London) 416, 155 (2002)
  4. V. Kiryukhin, D. Casa, J.P. Hill, B. Keimer, A. Vigliante, Y. Tomioka and Y. Tokura, "An x-ray-induced insulator-metal transition in a magnetoresistive manganite", Nature (London) 386, 813 (1997).

5. V. Kiryukhin, B. Keimer, J.P. Hill, S.M. Coad and D.M. Paul, Synchrotron x-ray scattering study of magnetic field induced transitions in  $\text{Cu}_{1-x}(\text{Zn,Ni})_x\text{GeO}_3$ ", Phys. Rev. B 54, 7269 (1996)

## Young S. Lee

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Massachusetts Institute of Technology  
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### Education

Princeton University	B.A., Department of Physics Certificate in Engineering Physics	1993 1993
Massachusetts Institute of Technology	Ph.D., Department of Physics Thesis title: "Neutron Scattering Study of the Magnetism and Structural Phases of Superconducting $\text{La}_2\text{CuO}_{4+y}$ " Advisor: Robert J. Birgeneau	2000

### Employment

11/1999 - 8/2001	NRC Postdoctoral Research Associate, NIST Center for Neutron Research
8/2001 - present	Assistant Professor, Department of Physics, Massachusetts Institute of Technology

### Professional Societies

American Physical Society, Neutron Scattering Society of America.

### Committees

Advanced Photon Source: Proposal Review Panel (Scattering, Condensed Matter).	2002 - present
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### Selected Publications:

- 1) K.J. Thomas, Y.S. Lee, F.C. Chou, B. Khaykovich, P.A. Lee, M.A. Kastner, R.J. Cava, and J.W. Lynn, “*Antiferromagnetism, ferromagnetism, and magnetic phase separation in  $\text{Bi}_2\text{Sr}_2\text{CoO}_{6+\delta}$* ” Phys. Rev. B **66**, 054415 (2002).
- 2) B. Khaykovich, Y.S. Lee, R.W. Erwin, S.H. Lee, S. Wakimoto, K.J. Thomas, M.A. Kastner, and R.J. Birgeneau, “*Enhancement of long-range magnetic order by magnetic field in superconducting  $\text{La}_2\text{CuO}_{4+y}$* ,” Phys. Rev. B **66**, 014528 (2002).
- 3) S. Wakimoto, R.J. Birgeneau, M.A. Kastner, Y.S. Lee, R.W. Erwin, P.M. Gehring, S.H. Lee, M. Fujita, K. Yamada, Y. Endoh, K. Hirota, and G. Shirane, “*Direct observation of a one-dimensional static spin modulation in insulating  $\text{La}_{1.95}\text{Sr}_{0.05}\text{CuO}_4$* ,” Phys. Rev. B **61**, 3699 (2000).
- 4) R.J. Birgeneau, M. Greven, M.A. Kastner, Y.S. Lee, B.O. Wells, Y. Endoh, K. Yamada, and G. Shirane, “*Instantaneous Spin Correlations in  $\text{La}_2\text{CuO}_4$* ,” Phys. Rev. B **59**, 13788 (1999).
- 5) Y.S. Lee, R.J. Birgeneau, M.A. Kastner, Y. Endoh, S. Wakimoto, K. Yamada, R.W. Erwin, S.H. Lee, and G. Shirane, “*Neutron Scattering Study of Spin Density Wave Ordering in the Superconducting State of Excess-Oxygen-Doped  $\text{La}_2\text{CuO}_{4+y}$* ,” Phys. Rev. B. **60**, 3643 (1999).
- 6) H. Kimura, K. Hirota, H. Matsushita, K. Yamada, Y. Endoh, S.H. Lee, C.F. Majkrzak, R.W. Erwin, G. Shirane, M. Greven, Y.S. Lee, M.A. Kastner, and R.J. Birgeneau, “*Neutron-scattering Study of Static Antiferromagnetic Correlations in  $\text{La}_{2-x}\text{Sr}_x\text{Cu}_{1-y}\text{Zn}_y\text{O}_4$* ,” Phys. Rev. B **59**, 6517 (1999).
- 7) Y.S. Lee, M. Greven, B.O. Wells, R.J. Birgeneau, and G. Shirane, “*Spin Correlations in the Two-Dimensional Spin-5/2 Heisenberg Antiferromagnet  $\text{Rb}_2\text{MnF}_4$* ,” Eur. Phys. J. B **5**, 15 (1998).
- 8) B.O. Wells, Y.S. Lee, M.A. Kastner, R.J. Christianson, R.J. Birgeneau, K. Yamada, Y. Endoh, and G. Shirane, “*Incommensurate Spin Fluctuations in High Temperature Superconductors*,” Science **277**, 1067 (1997).

## Stephen Eric Nagler

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### Personal Data:

Born: May 17, 1956, Calgary, Alberta  
Nationality: Dual citizen of the United States and Canada

### Education:

1978 B.Sc. (Physics) University of Toronto  
1982 Ph.D. (Physics) University of Toronto

### Professional Employment:

1995 - Research Staff Member, ORNL (Group Leader 1996 - )  
Adjunct Professor of Physics, University of Florida (1996 - )  
Adjunct Professor of Physics, University of Tennessee (1997 - )  
1984 – 1996 Professor of Physics, University of Florida, Gainesville, FL  
(Assistant Professor 1984 – 1989, Associate Professor 1989- 1993)  
1994 Visiting Scientist, Brookhaven National Laboratory  
1993 Visiting Professor, Weizmann Institute of Science, Rehovot, Israel  
1990 – 1991 Visiting Professor, Clarendon Laboratory, University of Oxford, UK  
1982 – 1984 Visiting Research Scientist, IBM Research, Yorktown Heights, NY

### Selected Honors and Awards:

Fellow of the American Physical Society  
ORNL Scientist of the Year 1998  
NSF Presidential Young Investigator Award 1986-92

### Selected Professional Activities:

Current Member, SNS Experimental facilities Advisory Committee  
NSERC College for review of Canada Research Chairs  
Chairman, Inelastic Scattering Subcommittee, IPNS PAC  
Recent Program Committee, American Conference on Neutron Scattering, 2002  
Publication Committee, SCES 2001  
Member, Blume Committee on Future of Neutron Scattering

### Selected Recent Publications:

- B. Lake, D.A. Tennant and S.E. Nagler, *A Novel Longitudinal Mode in the Coupled Quantum Chain Compound  $KCuF_3$* , cond-mat/9910459, PRL **85**, 832 (2000).
- W. Montfrooij, G.E. Granroth, D.G. Mandrus and S.E. Nagler, *Spin Dynamics of the Quasi-1D Ferromagnet  $CoCl_2 \cdot 2D_2O$* , PRB **64**, 134426 (2001).
- M.D. Lumsden, B.C. Sales, D.G. Mandrus, S.E. Nagler and J.R. Thompson, *Weak Ferromagnetism and Field-Induced Spin Reorientation in  $K_2V_3O_8$* , PRL **86**, 159 (2001).
- B.C. Sales, M.D. Lumsden, S.E. Nagler, D. Mandrus and R. Jin, *Magnetic Field Enhancement of Heat Transport in the 2D Heisenberg Antiferromagnet  $K_2V_3O_8$* , PRL **88**, 095901 (2002).
- S.E. Nagler, W.-T. Lee and R.M. Moon, *Design and Simulation of the CG1 Beamline at HFIR*, to be published in Applied Physics A (proceedings of ICNS 2001).

## Laurence Passell

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- Address:** Physics Department, Building 510B, Brookhaven National  
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- Education:** B.S. U.S. Merchant Marine Academy (1945)  
A.B. Harvard University (1950)  
M.A. University of California (Berkeley) (1952)  
Ph.D. University of California (Berkeley) (1955)  
Ph.D. thesis - Thermal Conductivity of Aluminum Below One  
Degree Absolute; thesis advisor - Professor H.B. Silsbee
- Employment:** Administration (1945-46) Assistant Port Engineer, U.S. War Shipping  
  
(1951) Los Alamos National Laboratory  
(1955-61) Lawrence Livermore Radiation Laboratory  
(1961-63) Risoe National Laboratory  
(1963-95) Brookhaven National Laboratory  
(1995-present) Brookhaven National Laboratory (consultant)
- Professional Societies:** American Physical Society (Fellow)  
Sigma Xi
- Committees:** SNS Neutron Optics Committee
- Awards and Honors:** Department of Energy 1998 Materials Science Award for  
Sustained Research in Materials Chemistry
- Publications:**
- The Performance of Reflecting Multi-Channel Collimators as Neutron Beam Filters and Polarizers; H.B. Moller, L. Passell and F. Stecher-Rasmussen - J. Nucl. En. 17, 227 (1963)
- Nuclear Polarization in EuS and EuO; L. Passell, V.L. Sailor and R.I. Schermer - Phys. Rev. 135A, 1767 (1964)
- Measurement of the Spin Dependence of the  $^3\text{He}(n,p)\text{T}$  Reaction and of the Susceptibility of Adsorbed  $^3\text{He}$ ; L. Passell and R.I. Schermer - Phys. Rev. 150, 146 (1966)
- Excitations in Few-Atomic-Layer Adsorbed Helium Films: The Two-Dimensional Roton; W. Thomlinson, J.A. Tarvin and L. Passell - Phys. Rev. Lett. 44, 266 (1980)
- Composite Germanium Monochromators for High Resolution Neutron Powder Diffraction Applications; J.D. Axe, S. Bar-Ziv, S. Cheung, D.E. Cox, L. Passell and T. Vogt - J. Neutron Res. 2, 85 (1994)

## REGNAULT Louis-Pierre

- Date of Birth:** February 4 1952
- Address:** CEA-Grenoble, 17 Rue des Martyrs 38054 Grenoble cedex 9, France  
Tel: +33438783137 Fax: +33438783137 e-mail: regnault@ill.fr
- Education:**
- o "Physics Master", University of Grenoble, 1974
  - o "D.E.A." in Solid State Physics, University of Grenoble, 1975.
  - o "3rd Cycle" thesis, University of Grenoble, 1976 (Title: "Ordre magnetique dans le compose a structure bidimensionnelle BaCo2As2O8"; Supervisor: J. Rossat-Mignod).
  - o Ph.D. Thesis, University of Grenoble, 1981 (Title: "Contribution a l'etude des excitations non-lineaires dans des systemes uni et bidimensionnels a anisotropie planaire"; Supervisor: J. Rossat-Mignod).
  - o Habilitation, 1985
- Employement:**
- 1976-1981 PhD at CEA-CENG-DRF, Neutron scattering laboratory (DRF/DN).
  - 1981 "Ingénieur" CEA . Responsible for the three-axes spectrometer (TAS) DN1 at the Siloé reactor, CEN-Grenoble.
  - 1991-1995 Adjoin director of the MDN laboratory at CEN-Grenoble.
  - Since 1995 Director of the MDN laboratory. Head of the CEA-"CRG" group at the ILL (D15, D23, IN12 and IN22).
  - 1995-1998 Leader of the "H25" Project (construction of a polarised neutron diffractometer (D23) and a polarised three-axis spectrometer with a longitudinal and a spherical polarisation analysis option (IN22) on a supermirror guide).
  - 1995-2002 First responsible of the "CRG" TAS IN22 at ILL.
- Professional societies:** Member of the French and European Physical Societies (SFP and EPS).  
Member of the French and Swiss Neutron Societies (SFN and SNS!).
- Committees and "networks":**
- Since 1999: Member of the ILL "working-group" on neutron polarimetry.
  - Since 2000 : Member of the ILL "Instrumentation subcommittee".
  - From 1996 to 2000: Member of the X-ENNI European network on neutron polarisation (Large area Heusler-based polarisers and polarisation-analysis devices for TAS; Spherical polarimetry for INS; Polarised neutron scattering under high magnetic fields).
  - Since 2000: Member of the ENPI (European Neutron polarisation Initiative) network (Construction of a third-generation "CRYOPAD" optimised for inelastic neutron scattering; Spherical polarimetry on TAS).
- Awards and Honors:** None. But my successive bosses got them for me!  
Since 2002 : "Directeur de Recherche" at CEA.

### Publications concerning polarised neutrons:

"Polarized neutron scattering on low-dimensional systems", L.P. Regnault, Proceedings of the "French-Japanese Symposium in Fukuoka, ed. Y. Ajiro and J.P. Boucher, (Kyushu University Press, 2002) 93-101.

- "Chiral criticality in helimagnet Ho studied by polarized neutron scattering", V.P. Plakhty, W. Schweika, Th. Bruckel, J. Kulda, S.V. Gavrilov, L.P. Regnault, and D. Visser, *Phys. Rev. B* **64** (2001) 100402-405.
- "Magnetization distribution in Si-doped spin-Peierls compound CuGeO<sub>3</sub>", B. Grenier, E. Ressouche, L.P. Regnault, J.E. Lorenzo, E. Lelievre-Berna, G. Dhalenne, and A. Revcolevschi. *Physica B* **297** (2001) 221-225.
- "Application des neutrons polarisés à l'étude des excitations magnétiques", L.P. Regnault, *J. Phys. IV France* **11** (2001) 253-269.
- "Antiferromagnetic ordering in superconducting YBa<sub>2</sub>Cu<sub>3</sub>O<sub>6.5</sub>", Y. Sidis, C. Ulrich, P. Bourges, C. Bernhard, C. Niedermayer, L.P. Regnault, N.H. Andersen, and B. Keimer, *Phys. Rev. Lett.* **18** (2001) 4100-4103.
- "Coupled magnetic and structural transitions in EuMn<sub>2</sub>O<sub>5</sub> as studied by neutron diffraction and three-dimensional polarization analysis", V. Polyakov, V. Plakhty, M. Bonnet, P. Burlet, L.P. Regnault, S. Gavrilov, I. Zobjkalo, and O. Smirnov, *Physica B* **297** (2001) 208-212.
- "The current status of the <sup>3</sup>He neutron spin filter (NSF) project at the ILL", T.W. Roberts, H. Humblot, F. Tasset, E. Lelièvre-Berna, A.R. Wildes, A. Ivanov, A. Petoukhov, L.P. Regnault, A.D. Hiller, J. Kulda, J.R. Stewart, M. Thomas, P. Malbert, D. Jullien, Y. Gibert, P. Gay, E. Bourgeat-Lami, and R. Chung, *Physica B* **297** (2001) 282-287.
- "Cryopol: a superconducting magnetostatic cavity for a <sup>3</sup>He neutron spin filter", J. Dreyer, L.P. Regnault, E. Bougeat-Lami, E. Lelièvre-Berna, S. Pujol, F. Thomas, M. Thomas, F. Tasset, *Nuclear Instrumentation and Methods A* **449** (2000) 638-648.
- "Incommensurate antiferromagnetic fluctuations in superconducting YBa<sub>2</sub>Cu<sub>3</sub>O<sub>6.85</sub>", H.M. Ronnow, L.P. Regnault, C. Ulrich, B. Keimer, P. Bourges, and Y. Sidis, ILL Annual Report 2000 (<http://www.ill.fr/AR-00/scientific.htm>).
- "Polarized neutron inelastic scattering on the spin-Peierls system CuGeO<sub>3</sub>: "three-directional" versus "three-dimensional" polarisation analysis", L.P. Regnault, F. Tasset, J.E. Lorenzo, T. Roberts, G. Dhalenne, and A. Revcolevschi, *Physica B* **267-268** (1999) 227-235.



## James J. Rhyne

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11/14/1938
- Address:** Physics Dept., Univ. of Missouri, Columbia, MO 65211  
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- Education:**
- Ph.D. in Physics, Iowa State University, 1965, Thesis Title: *Magnetostriction in Rare Earth Metals*, S. Legvold, thesis supervisor
  - M.S. in Physics, University of Illinois, 1961
  - B.S. in Physics (with honors), University of Oklahoma, 1959
- Employment (partial list):**
- Research Physicist, Solid State Division, Naval Ordnance Laboratory (NOL), 1965-1975.
  - Research Physicist, Reactor Radiation Division, National Institute of Standards and Technology (NIST), 1975-1990
  - Visiting Scientist, Riso National Laboratory, Roskilde, Denmark, 1978.
  - Director, NSF/NIST Center for High Resolution Neutron Scattering, National Institute of Standards and Technology (formerly the National Bureau of Standards), 1988-1990.
  - Director, University of Missouri Research Reactor Center, 1991 – 1996
  - Professor, Department of Physics, University of Missouri-Columbia, 1991 - present.
  - Faculty Appointment, Reactor Radiation Division, NIST, January 1991-September 1995; Guest Worker, October 1995-present.
- Professional Societies:**
- Fellow, American Physical Society and Washington Academy of Sciences
- Committees (partial list):**
- President, Neutron Scattering Society of America, elected 1999 (3 year term)
  - Member, Executive Committee, GMAG, American Physical Society, elected 1999 (3 year term)
  - Member, Basic Energy Sciences Advisory Committee, Subpanel on Neutron Sources, 2000.
  - Advisory Editor, Journal of Magnetism and Magnetic Materials, 1990-present.
  - Chair, Neutron Instrumentation Panel, DOE Facilities Initiative Review, Chantilly, VA, May 1-2, 1996.
  - Member, Intl. Atomic Energy Agency (IAEA) Advisory Group on *Use of Research Reactors for Solid State Studies*, Vienna, Austria, March 29-April 1, 1993.
  - Member, Scientific Committee, Louis Néel Laboratory, C.N.R.S., Grenoble, France, 1989-1991.
  - Delegate to the Megascience Forum on Neutron Sources sponsored by the International Organization for Economic Cooperation and Development, Knoxville, November 1994.
  - Member, National Steering Committee, Advanced Neutron Source Project, 1992-1995.

- Member, Advisory Committee, Los Alamos Neutron Scattering Center, 1991 - 1994.
- Chairman, Program Review Committee, Argonne and Los Alamos National Laboratories Pulse Neutron Sources, 1989; Member 1986-1989.
- Member, Editorial Board, Journal of Applied Physics, 1986-1989.
- Publications Chairman and Member Executive Committee, 1985 International Conference on Magnetism, 1981-1985.

**Awards and Honors:**

- Doctor Honoris Causa, University Henri Poincaré, Nancy, France, conferred June 20, 1995
- Fellow, American Physical Society and Washington Academy of Sciences
- Department of Commerce Gold Medal Award, 1987; Silver Medal Award, 1984
- National Bureau of Standards Bronze Medal Award, 1981

**Publications (partial list):**

- “Spin Dynamics And Absence Of A Central Peak Anomaly In  $\text{La}_{0.67}\text{Ca}_{0.33}\text{MnO}_3$ ,” J.J. Rhyne, H. Kaiser, L. Stumpe, J.F. Mitchell, T. McCloskey, and A.R. Chourasia, *J. Appl. Phys.* **87**, 5813 (2000).
- “Composition dependence of the spin wave stiffness parameter in  $\text{La}_{1-x}\text{Ca}_x\text{MnO}_3$  CMR materials,” J.J. Rhyne, H. Kaiser, L. Stumpe, J.F. Mitchell, T. McCloskey, and A.R. Chourasia, *J. Mag. And Mag. Matls.* **226-230**, 775 (2001).
- “Spin Excitations in  $[\text{La}_{1-x}\text{Ca}_x\text{MnO}_3]$  in the Mixed-Phase Region,” L. Stumpe, B. Kirby, H. Kaiser, J.J. Rhyne, and J.F. Mitchell, *J. Appl. Phys.* **91**, 7511 (2002).
- “Long Wavelength Spin Dynamics in  $\text{La}_{0.53}\text{Ca}_{0.47}\text{MnO}_3$ ,” J.J. Rhyne, H. Kaiser, H. Lao, Gang Xiao, and M.L. Gardel, *J. Appl. Phys.* **83**, 7339 (1998).
- “Concurrent Nd and Mn Spin Excitations in  $\text{Nd}_{0.6}\text{Sr}_{0.4}\text{MnO}_3$ ,” H. Kaiser, L.E. Stumpe, J. J. Rhyne, Y. Tokura, and H. Kuwahara,” *J. Appl. Phys.* **85**, 5564 (1999).
- “Small Angle Neutron Scattering of Nanodispersed Magnetic Particles,” J.R. Childress, C.L. Chien, J.J. Rhyne, and R.W. Erwin, *J. Mag. and Mag. Matls.* **104-107**, 1585 (1992).
- “Neutron Scattering Study of the Magnetic Correlations of Iron-Rich Fe-Ni-Zr Glasses,” J.A. Fernandez-Baca, J.J. Rhyne, R.W. Erwin and G.E. Fish, *J. de Physique, Colloque C8, Suppl. #12*, **49**, 1207 (1988).
- “Magnetism in Artificial Metallic Superlattices of Rare Earth Metals,” J. J. Rhyne and R. W. Erwin, Chapt. 1, *Handbook of Magnetic Materials*, Vol. 8, edited by K.H.J. Buschow, North Holland Science Publishers, pp. 1-56 (1995).
- “Spin Dynamics of Amorphous Magnets,” J.W. Lynn and J.J. Rhyne, Chapter 14, *Spin Waves and Magnetic Excitations*, Vol. 2, edited by S.K. Sinha and A.S. Borovik-Romanov, North Holland Physics Publishers, Amsterdam, 1988, pp. 177-217.

## Constantine J. Stassis

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- Education:**
- B.S. Physics, 1960, École Polytechnique de l' Université de Lausanne, Switzerland
  - M.S. Physics, 1961, École Polytechnique de l' Université de Lausanne, Switzerland
  - Ph.D. Physics, 1970, Massachusetts Institute of Technology (MIT), USA  
thesis: "Polarized Neutron Study of Nagaoka's Quasibound State"  
thesis supervisor: Prof. C. G. Shull (deceased)
- Employment:**
- 1970: Post-doctoral Research Associate, MIT
  - 1971: Instructor, Iowa State University and Assistant Physicist Ames Laboratory
  - 1972: Assistant Professor, Iowa State University and Associate Physicist Ames Laboratory
  - 1975: Associate Professor, Iowa State University and Physicist Ames Laboratory
  - 1979-present: Professor of Physics, Iowa State University and Senior Physicist Ames Laboratory
  - 1987: Visiting Scientist, Brookhaven National Laboratory
  - 1989: Visiting Scientist, Brookhaven National Laboratory
  - 1987-1988: Visiting Professor of Physics, University of Crete, Greece
  - 1996: Summer Visiting Scientist, Brookhaven National Laboratory
- Professional Societies:** Member, American Physical Society; Fellow, American Physical Society; Member, Neutron Scattering Society of America (NSSA); Member, Executive Committee and Membership Secretary of the Neutron Scattering Society of America (NSSA)(1993-present); Member, Joint Spallation Neutron Source (SNS) and High Flux Isotope Reactor (HFIR) Users Committee (SHUC)(1998-present).
- Awards and Honors:** 1997 Co-recipient of the DOE Annual Award for Outstanding Accomplishments in Solid State Physics.
- Publications:**
- J. Zarestky, C. Stassis, A. Goldman, P. Canfield, G. Shirane, S.M. Shapiro, "Phonon-Phonon Interactions in (Lu,Y)Ni<sub>2</sub>B<sub>2</sub>C," *J.Phys.Chem.Sol.*, **63**, 811 (2002).
- Ll. Mañosa, Antonio Planes, J. Zarestky, T. Lograsso, D.L. Schlagel, C. Stassis, "Phonon Softening in Ni-Mn-Ga alloys" *Phys. Rev. B*, **64**, p. 024305 (2001).
- C. Stassis, "Neutron Scattering," Chapter 17 in *Handbook of Elastic Properties of Solids, Liquids and Gases*, Academic Press (New York, NY) (2001).
- I.R. Fisher, Z. Islam, J. Zarestky, C. Stassis, M.J. Kramer, A.I. Goldman and P.C. Canfield, "Magnetic

Properties of Icosahedral R-Mg-Zn quasicrystal (R=Y, Tb, Dy, Ho and Er) *J. Alloys Compd.* **303-304**, 223 (2000).

C. Stassis, "Techniques for the Study of Phonons," Section 14.7 in *Methods of Materials Research*, John Wiley and Sons, Inc. (2000).

S. H. Lee, C. F. Majkzszak, S. K. Sinha, C. Stassis, H. Kawano, G. Lander, P. Brown, H. F. Fong, S. W. Cheong, H. Matsushita, K. Yamada, Y. Endoh, "Search for Orbital Moments in Underdoped Cuprate Metals – A Sisyphean Experience," *Phys. Rev. B* **60**, 10405 (1999).

J. Zarestky, C. Stassis, A. Goldman, P. Canfield, G. Shirane, S. Shapiro, "Phonon Profiles in Superconducting  $\text{YNi}_2\text{B}_2\text{C}$  and  $\text{LuNi}_2\text{B}_2\text{C}$ ," *Phys. Rev. B* **60**, 11932 (1999).

C. Stassis, J. Zarestky, A. Goldman, P. Canfield, G. Shirane, S. Shapiro, "Anomalous Phonons Below  $T_c$  in Superconducting  $\text{RNi}_2\text{B}_2\text{C}$  (R = Lu, Y)," *Physica C* **317-318**, 127 (1999).

## Andrey Zheludev

### Curriculum Vitae

<b>Place and date of birth:</b>	Moscow, Russia, October 17, 1969
<b>Address</b>	Oak Ridge National Laboratory Building 7962, MS 6393 P.O. Box 2008 Oak Ridge, Tennessee 37831-6393
<b>Education</b>	
1994	<b>Ph.D.</b> in Physics, <i>summa cum laude</i> , Université Joseph Fourier, Grenoble, France. <u>Title</u> : "Etudes de cristaux magnetique moleculaires par diffraction de neutrons." <u>Supervisor</u> : Dr. J. Schweizer, CEA Grenoble.
1991	<b>M.S.</b> in Physics, <i>summa cum laude</i> , Moscow Institute for Physics and Technology (MIPT) and the P.L.Kapitza Institute for Physical Problems, Russian Acad. Sci. (IPP), Moscow, Russia
1991	<b>M.S.</b> in Applied Mathematics, <i>summa cum laude</i> , MIPT and IPP
1989	<b>B. S.</b> in Physics, Faculty of General and Applied Physics, MIPT, Moscow, Russia
1989	<b>B.S.</b> in Mathematics, MIPT, Moscow, Russia
<b>Employment</b>	
2001-Present	Research Staff II, Solid State Division, Oak Ridge National Laboratory
2000-2001	Physicist, Physics Department, Brookhaven National Laboratory
1998-2000	Associate Physicist, Physics Department, BNL
1996-1998	Assistant Physicist, Physics Department, BNL
1994-1996	Research Associate, Physics Department, BNL
1991-1994	Junior Research Associate, Centre d'Etudes Nucleaires de Grenoble, France
1991-1993	Junior Research Associate, P.L.Kapitza Institute for Physical Problems, Russian Acad. Sci., Moscow, Russia
<b>Membership in professional associations</b>	
1994-1999, 2002-present	American Physical Society
1996-present	Neutron Scattering Society of America

## Honors and awards

2000	2000 The Presidential Early Career Award For Scientists and Engineers. 2000 US DOE Office of Science Early Career Scientist and Engineer Award.
1997	INS approval of permanent US residency petition filed by Brookhaven National Laboratory under the category “Outstanding ability”.
1993	CEA (France) award for “Prominent Research Achievements in Condensed Matter Physics” for work on New Organic Magnetic Materials.
1986-1991	Fellowship for Outstanding College Students, MIPT.

## 10 selected recent publications in neutron scattering

A. Zheludev, K. Kakurai, T. Masuda, K. Uchinokura, K. Nakajima, *Dominance of excitation continuum in the longitudinal spectrum of weakly coupled Heisenberg  $S=1/2$  chains*, Phys. Rev. Lett. **89**, 197205 (2002).

A. Zheludev, Z. Honda, Y. Chen, C. L. Broholm, K. Katsumata, S. M. Shapiro, *Gapless excitations in the high-field phase of a Haldane antiferromagnet*, Phys. Rev. Lett **88**, 077206 (2002).

A. Zheludev, E. Ressouche, I Tsukada, T. Masuda and K. Uchinokura, *Structure of the multiple spin-flop states in BaCu<sub>2</sub>Si<sub>2</sub>O<sub>7</sub>*, Phys. Rev. B **65**, 174416 (2002);

A. Zheludev, M. Kenzelmann, S. Raymond, T. Masuda, K. Uchinokura, S.-H. Lee, *Spin dynamics in the  $S=1/2$  weakly-coupled chains antiferromagnet BaCu<sub>2</sub>Si<sub>2</sub>O<sub>7</sub>*, Phys. Rev. B **65**, 014402 (2001).

A. Zheludev, S. Maslov, T. Yokoo, J. Akimitsu, S. Raymond, S. E. Nagler, *Quantum and classical dynamics in complex one-dimensional antiferromagnets*, J. Phys.: Condens. Matter **1**, R525-R536 (2001).

Y. Chen, Z. Honda, A. Zheludev, C. Broholm, K. Katsumata and S. M. Shapiro, *Field-induced 3- and 2-dimensional freezing in a quantum spin liquid*, Phys. Rev. Lett. **86**, 1618 (2001).

A. Zheludev, Z. Honda, K. Katsumata, R. Feyerherm and K. Prokes, *Field-induced commensurate long-range order in the Haldane-gap system Ni(C<sub>5</sub>H<sub>14</sub>N<sub>2</sub>)<sub>2</sub>N<sub>3</sub>(ClO<sub>4</sub>)*, Europhys. Lett. **55**, 868 (2001)

A. Zheludev, M. Kenzelmann, S. Raymond, E. Ressouche, T. Masuda, K. Kakurai, S. Maslov, I. Tsukada, K. Uchinokura, A. Wildes, *Energy separation of single-particle and continuum states in a  $S=1/2$  weakly-coupled chain antiferromagnet*, Phys. Rev. Lett., **85**, 4799 (2000).

Y. Uchiyama, Y. Sasago, I. Tsukada, K. Uchinokura, A. Zheludev, T. Hayashi, N. Miura and P. Boni, *Spin-Vacancy-Induced Long-Range Order in a New Haldane-Gap Antiferromagnet*, Phys. Rev. Lett., **83**, 632 (1999).

A. Zheludev, S. Maslov, G. Shirane, I. Tsukada, T. Masuda, K. Uchinokura, I. Zaliznyak, R. Erwin, L. P. Regnault, *Magnetic anisotropy and low-energy spin waves in the Dzyaloshinskii-Moriya spiral magnet Ba<sub>2</sub>CuGe<sub>2</sub>O<sub>7</sub>*, Phys. Rev. B **59**, 11432 (1999).

## Appendix B. SNS Document: IS-1.1.8.2-8004-MM-A-00 (selected pages)

A group of researchers representing several disciplines met at Argonne National Laboratory to establish scientific priorities for the inelastic neutron scattering instruments to be available at the SNS at the beginning of operations. The Workshop consisted of breakout sessions into three groups representative of different user communities for inelastic scattering: i) magnetism, ii) thermodynamics, lattice effects, and critical phenomena, and iii) chemical spectroscopy. A joint meeting of all three groups to discuss common interests and explore the overall needs for instrumentation followed. This report summarizes these discussions.

The report is organized as follows: Section I enumerates the instruments considered for inclusion in the Inelastic Scattering suite of instruments for SNS. Sections II(A,B,C) report on the scientific needs identified in the breakout sessions. Section III consists of a summary and the recommendations of the working groups.

### I. Instruments

The instruments considered were broken up into three categories as summarized in table I below. Category A consists of instruments already identified by the SNS Instrument Oversight Committee as high priorities for study and design. Additional instruments, denoted by category B, have been identified for priority consideration at this Workshop. Other instruments which also should be discussed are in category C. The instruments in Table I are labeled by category letters and numbers. The numbers are for convenience of discussion only and do not reflect priorities. Further details of the instruments are discussed in sections II and III.

Table I : Instruments Discussed

Category	Instrument
A.1	indirect geometry spectrometer, (backscattering), resolution 2 $\mu\text{eV}$ (elastic position)
A.2	Direct geometry spectrometer (chopper), resolution $\Delta E/E \sim 1\%$ (elastic position), $E \sim 10 - 1000$ meV, continuous angular coverage
A.3	Spectrometer with 10 – 100 $\mu\text{eV}$ resolution
B.1	Chopper, $\Delta E/E \sim 5\%$ (elastic position), large angular coverage
B.2	Inverse geometry spectrometer, time focussed, $\Delta E/E \sim 1\%$
B.3	Triple axis-like instrument with high signal to noise
B.4	High Q chopper spectrometer with small $\Delta E/E$
C.1	Spin echo spectrometer $\Delta E \sim 1$ neV to 2 $\mu\text{eV}$
C.2	Brillouin scattering spectrometer, small Q, intermediate E
C.3	PRISMA-like spectrometer

a large number of analytical techniques in common use in chemistry, such as optical spectroscopy, nuclear magnetic resonance, electron spin resonance, and gas chromatography/mass spectroscopy. For example, the ability to simultaneously measure diffusion using magnetic resonance techniques and quasielastic neutron scattering would provide for an unprecedented ability to measure diffusion over many orders of magnitude on the same sample.

The most logical way forward for the development of such multiple probe techniques is to develop the concept of a “sample environment module” which can be assembled with the desirable options and samples. This would be done outside of the instrument, leading to greater control and reproducibility, and more importantly avoid the considerable waste of beam time which occurs during sample “preparation” (e.g. cooling, heating, irradiation with lasers etc.). This is likely to be a major issue with some of the faster instruments envisaged for the SNS.

For all three types of scattering the abilities to go to pressures of 0.1 Gpa was considered useful, as was continuous and pulsed ( $> 10\text{Hz}$ ) magnetic fields (i.e., fields as high as possible, but consistent with the need for an acceptable count-rate). Furnaces capable of providing sample temperatures for measurements up to 2000K are also desirable, in addition to the more conventional cryogenic equipment capable of going down to about 1K. For quasielastic scattering, a shear cell will provide the novel ability to measure transport properties as a function of shear.

Finally, the issue of small samples needs to be addressed using neutron optical elements to focus the beam onto small volumes. It is also desirable to provide a polarized neutron option, in order to discriminate between coherent and incoherent scattering from complex materials.

### **III. Summary and Recommendations**

After the breakout sessions of the three working groups, a general discussion session was convened to discuss the overall needs for inelastic scattering instrumentation at the SNS. The various science-based criteria were evaluated in the light of the likely capabilities of different types of neutron spectrometer designs (e.g., direct geometry and inverse geometry instruments). This discussion led to consideration of the 10 instruments listed in Table I.

The SNS project currently has three ongoing or planned design studies for new spectroscopy instruments for “day-one” operation of the SNS. These are listed in Table I, section A. On the basis of the scientific requirements articulated by the working groups, these three instruments are desirable to address a wide variety of scientific problems. After further discussion it was decided that a total of seven instruments, those listed in Table I-A and I-B, should be studied as potential “day-one” instruments.

The three remaining instruments (Table I-C) are not being recommended for further study at this time. The spin-echo spectrometer is desirable for a wide variety of scientific applications but there is the prospect that a SNS-Julich/HMI collaboration will



## Appendix C. HYSPEC Top Level Specifications.

This document defines “top-level” requirements for all components of the hybrid spectrometer, HYSPEC, planned for installation on beamline 15 (BL15) of the Spallation Neutron Source (SNS) that is now under construction at Oak Ridge National Laboratory. All HYSPEC components, whether designed by the Instrument Development Team (IDT), members of the SNS staff, or by third party manufacturers, are expected to comply with these requirements. It becomes effective only if signed by all of the parties whose names appear below. Changes and additions (or deletions) can be initiated by any of the signatories (or their replacements) at which time a revised document must be prepared with all modified sections identified as such. They become effective only after all parties sign the revised document. Whenever revisions are made, the earlier document is to be retained as part of the IDT record.

Principal Investigator:	S. Shapiro	.....,	Date .....
Principal Investigator:	I. Zaliznyak	.....,	Date .....
Project Scientist:	TBA	.....,	Date .....
SNS Instrument Systems:	K. Crawford	.....,	Date .....
SNS EFD Head:	I. Anderson	.....,	Date .....
SNS Director:	T. Mason	.....,	Date .....

Requirements for HYSPEC.<sup>(1)</sup>

## 1. Instrument footprint and placement on the floor.

HYSPEC shall be placed at the end position of the SNS beam-line illuminated by a coupled, supercritical H<sub>2</sub> moderator. Sufficient floor space must be available at this position to accommodate the instrument's secondary spectrometer for all incident energies and sample scattering angles specified in sections 3 and 5 below. The greater part of the instrument footprint will be a 6.3 m radius semi-circle, on one side of the beam-line or the other. It will be centered at the monochromator position, at a distance L<sub>SM</sub> of about 20 to 25 m from the moderator face; nominal moderator-to-monochromator distance L<sub>SM</sub> = 20000 mm is used in this document. It is assumed that this semi-circular footprint shall be entirely inside the SNS experimental hall. A combined "get-lost" pipe and beam-stop – if they prove to be necessary – may extend outside the building.

It is currently envisioned that HYSPEC will be located on BL15, behind a shorter instrument served by an ambient water moderator on BL16A. Should SNS Instrument Team judge that spectrometer footprint cannot be accommodated on BL15 in accordance with the above requirements a mutually acceptable alternative shall be negotiated between the HYSPEC IDT and the SNS. The possible alternatives, in the IDT order of preference, are: (i) HYSPEC reassignment to another beam-line served by a coupled, super-critical H<sub>2</sub> moderator, such as BL14B; (ii) slight modification of the instrument design by reducing the secondary flight-path: the energy resolution is relaxed proportionally, but the footprint is reduced also; this, however, may also impact the polarization sensitivity; (iii) complete re-design of the instrument secondary spectrometer so that the longest secondary flight-path available for each scattering angle is used, as a result the footprint becomes elongated and "pear-shaped"; (iv) extending the spectrometer primary flight-path to a building outside the SNS experimental hall; at a given analyzer resolution this reduces the incident neutron flux in proportion to the length of the primary spectrometer, and, while being more expensive, is somewhat equivalent to reducing the secondary flight-path.

## 2. Primary flight-path system

### 2.1 Neutron guide system

The incident neutron guide system is to be composed of three super-mirror guide sections, **G1-G3**, all with top and bottom coatings with critical angles of  $3\theta_c^{\text{Ni}}$  and with side coatings with the largest practical critical angle larger than  $3\theta_c^{\text{Ni}}$ . **G1** is to be integrated into the primary shutter. So located, its upstream end with an internal aperture of  $w_o \times h_o = 40 \text{ mm} \times 128 \text{ mm}$  will be at a distance  $L_0 = 2000 \text{ mm}$  from the front face of the coupled, supercritical H<sub>2</sub> moderator. Gaps of the smallest possible size are to be provided in the guide system to accommodate shutter, choppers and (if necessary) a beam filter assembly. **G2** and **G3**, the sections external to the biological shield, are to be steel-jacketed. All guide sections shall be 40 mm wide; their internal vertical profiles will be chosen to optimize the neutron current illuminating the 240 mm tall, vertically-focusing

monochromator crystal that will be located downstream of **G3** at a distance of  $L_{SM} = 20000$  mm from the front face of the moderator. Optimization is to be achieved at a reference incident neutron energy  $E_i = 15$  meV. Existing Monte-Carlo simulations indicate that the optimum guide dimensions are:

Guide section	Length	Entrance size, $w \times h$	Exit size, $w \times h$
<b>G1</b>	5000 mm	40 mm x 128 mm	40 mm x 150 mm
<b>G2</b>	11000 mm	40 mm x 150 mm	40 mm x 150 mm
<b>G3</b>	2000 mm	40 mm x 150 mm	40 mm x 180 mm

These dimensions will be further refined as design work proceeds, however, and might, at a later stage, differ slightly from the above values.

The guide support system should be designed to allow easy alignment of the individual guide segments (both vertically and laterally) with positional precision better than 0.5 mm and angular precision better than 1 minute of arc.

To the extent feasible, the primary flight path sections should be either evacuated or filled with  $^4\text{He}$  gas to minimize air scattering losses.

## 2.2 Beam line shielding

Beam line shielding shall consist of a stationary bottom piece carrying the guide support and alignment systems and removable modular pieces on the sides and top. The removable shielding is to be designed so as to: (i) minimize the space immediately surrounding the guide system (as specified in section 2.1) that is not filled with shielding material; (ii) minimize the total thickness and weight of the modular shielding and (iii) provide rapid and convenient access to the choppers and (if installed) filters for maintenance and, if necessary, for their removal. Shielding shall be composite and contain materials needed both to slow down and absorb neutrons and to absorb the prompt gamma radiation. Radiation dose rates and background outside the beam line shielding shall be as low as reasonably achievable (ALARA); less than 5 mR/hr and in compliance with the limits established by the SNS.

## 2.3 Shutter

The primary beam shutter for the instrument shall be the SNS shutter inside the biological shield. When closed it must reduce the radiation incident on the choppers and monochromator crystal sufficiently to allow them to be removed for repairs while the SNS is operating at full power and also reduce the radiation level at the sample position to less than 5 mR/hr. The **G1** section of guide is to be built into the "open" channel of the shutter, as specified in section 2.1. Shutter position shall be controlled by a single switch interlocked to form a radiation exclusion zone details of which are to be specified by SNS. A clearly visible sign will show the shutter position; this information shall also be available to the instrument control computer. Shutter opening and closing times are to be less than 30 sec.

## 2.4 Filters

If MCNP-X based neutronics calculations indicate that single crystal beam filters can significantly reduce fast neutron beam contamination, a three-position filter exchanger is to be positioned immediately downstream of the in-shield shutter.

The filters are to be large enough in their lateral dimensions to intercept the full beam as specified in section 2.1. Each filter shall have the same supermirror coatings and shielding as the **G1** guide so that neutrons must either pass through the filter or be absorbed in the surrounding shielding. A refrigerator system should be provided to cool the filters to 77 K (or colder) and maintain them at that temperature even when fully illuminated by the neutron beam. Filter transmission better than 60% for neutrons throughout the energy range  $5 < E_i < 90$  meV is defined as being acceptable. Filter changes are to be effectuated from the instrument control computer. The filter choices shall be:

- 2.4.1 **None:** An open channel with lateral dimensions that accommodate the full beam as specified in 2.1.
- 2.4.2 **Sapphire:** Single crystal sapphire grade B4 or better with a beam path length of 100 mm (available from Crystal Systems Inc.). The orientation of the single crystal material is to be uniform throughout the filter to within 10 degrees. However, the average crystal orientation with respect to the beam direction is unimportant and should be chosen to minimize cost.
- 2.4.3 **PG:** Pyrolytic graphite grade ZYH with a total beam path length of 100 mm (available from Advanced Ceramics). The c-axes of the individual crystal plates must be aligned to within 2 degrees of the local beam axis.

### 3. Monochromating system

#### 3.1 General principle

Incident neutron energy selection in HYSPEC shall be defined by the combined effects of time-of-flight (TOF) along the primary flight-path and Bragg reflection from the monochromator crystal. TOF energy selection relies on restricting the burst time  $\tau_0$ ; i.e. the time interval during which the sample is illuminated by the incident neutron beam. A counter-rotating disc chopper pair, **T<sub>2</sub>**, positioned as close as possible to the upstream face of the monochromator crystal is to be used to define burst times  $\tau_0 > 50$   $\mu$ s. An additional “rotating collimator”-type Fermi-chopper, **T<sub>3</sub>**, operating at high rotation speeds shall be used in those cases where shorter burst times are needed. It is to be placed at the downstream end of the converging supermirror guide **G4** between the monochromator crystal and the sample, as described in section 3.5.

Crystal monochromator with variable vertical curvature shall serve to vertically focus the 240 mm tall neutron beam delivered by the guide system onto a sample placed in the beam center at a distance  $L_{MS}$  from the monochromator rotation axis. The crystals will also serve as pulse-shapers, cutting off much of the unwanted higher-energy tail from the spectral distribution of neutrons produced by the moderator. Pyrolytic graphite crystals will be used for most unpolarized beam applications although in certain cases where very low incident neutron energies are needed fluorinated synthetic mica crystals may be employed. For polarized beam studies, a vertically-focusing Heusler alloy crystal monochromator will be used to provide polarized monochromatic neutrons incident on the sample. The monochromator crystals shall be mounted in fixtures

such that they can be remotely aligned and also remotely rotated around a vertical axis to define the “take-off” angles needed to Bragg reflect neutrons with energies in the nominal range  $2.5 < E_i < 100$  meV.

A sample position arm rotating around the monochromating crystal shall connect the monochromator axis and the sample stage with its alignment and rotation axes. The arm shall hold a converging super-mirror guide, a Fermi chopper, a collimator, an incident beam monitor, beam defining slits, beam attenuators (including a beam shutter), and a polarized beam equipment such as a guide field and flipper for polarized applications. It shall be rigidly attached to the rotating exit aperture in the monochromator crystal shielding in such a way that the sample is always at the center of the monochromatic neutron beam reflected by the crystal. The converging super-mirror guide, Fermi-chopper and collimator are all to be contained within the monochromator shielding. Distances from the monochromator to the sample,  $L_{MS}$ , and to the upstream counter-rotating chopper pair,  $L_{TIM}$ , should be minimized while maintaining all other specifications. In normal operation the nominal value for  $L_{MS}$  is assumed to be 1800 mm.

### 3.2 Disk choppers

Three disk choppers designated  $T_0$ ,  $T_1$  and  $T_2$  rotating about their horizontal axes at a multiple or sub-multiple of the source frequency and kept very precisely in phase with the source shall be installed in the primary flight-path. All should fit as tightly within the gaps between guide sections as possible, housed in SNS approved, blast-proof housings, and should have neutron-transparent windows which, as the chopper rotate, provide time-dependent and uniform vertical illumination of the full downstream guide apertures as specified in section 2.1. Beam transmission should be at least 98% in the chopper “open” positions for neutrons with energies in the range  $2.5 < E_i < 100$  meV; a minimum beam attenuation of  $10^{-5}$  in the chopper “closed” position is defined as being acceptable. To the extent feasible, chopper modules shall be based on the standard designs developed by the SNS Instrument Systems Group. Because choppers are significant sources of scattering, additional modular shielding is to be placed around the beam-line at each chopper position to reduce radiation leakage to acceptable levels as specified in section 2.2.

- 3.2.1  **$T_0$  chopper:** A chopper with a highest rotation rate of 120 Hz and a lowest rotation rate 30 Hz made of a material that efficiently blocks fast neutrons and gamma-rays from the moderator is to be placed as close as possible to the moderator shielding face or possibly inside it. This chopper must block prompt fast neutrons and gamma rays but be open to neutrons in the energy range  $2.5 < E_i < 100$  meV. Also its “open” channel should be supermirror-coated and of the same lateral dimensions specified in section 2.1 for the surrounding guide so that the downstream guide is fully illuminated when the chopper is open.
- 3.2.2  **$T_1$ , the order-suppressing and frame-overlap chopper:** This chopper is to be a 300 mm radius, single rotor disc chopper with a highest rotation rate of 240 Hz and a lowest rate of 30 Hz. It shall be located either between guide sections **G1** and **G2**, or in a gap in **G2**. The chopper

should be designed to remove all unwanted higher-order neutrons that could otherwise pass through the  $T_2$  chopper (when operating at high rotation speeds) and be reflected by the monochromator crystal. In cases where frame overlap contamination becomes a problem either this chopper or the  $T_0$  chopper (or both) should be capable of being operated at half the source frequency (30 Hz) to block alternate pulses from the moderator.

- 3.2.3  **$T_2$ , the energy-defining chopper:** This is a double-rotor chopper composed of a pair of the counter-rotating 300 mm radius disk choppers with a highest operational rotation rate of 360 Hz. It should be placed as close as practical to the front face of the monochromator crystal, either between guide sections **G2** and **G3** or in a gap in guide **G3**.

### 3.3 Monochromator crystal assemblies

HYSPEC shall have two or more vertically focusing, segmented crystal monochromators mounted on a remotely-controlled exchanger; one shall be of pyrolytic graphite (PG) and one of Heusler alloy. Optional additional monochromator crystals based on intercalated PG, synthetic mica, silicon or germanium will be specified at a later stage. Their design is to be based on standard GMI-type segmented frames with a single-motor-driven mechanism to vary vertical curvature. Individual crystal segments shall be attached to aluminum alloy plates of the minimum practical thickness using aluminum screws or pins. All monochromator crystal assemblies should be of dimensions  $w_m \times h_m = 240 \text{ mm} \times 240 \text{ mm}$  so as to accommodate the full size of the neutron beam exiting guide **G3** for all scattering angles  $20^\circ < 2\theta_m < 120^\circ$ . All parts of the monochromator frame and its support and crystal exchange mechanisms and such other components as a magnetic yoke to provide the field needed to saturate the Heusler crystals are to be covered with a neutron-absorbing material such as  $B_4C$  and/or LiF. It should be possible to remove either or both monochromating crystal assemblies from the instrument for service while the SNS is in full power operation. A web camera with appropriate lighting shall be provided to enable remote viewing of the monochromators for diagnostic purposes when they are moved.

- 3.3.1 **PG monochromator:** shall be assembled of  $3 \times 60 = 180$  individual rectangular plates of ZYA grade pyrolytic graphite (from Advanced Ceramics or another vendor) with an isotropic intrinsic (x-ray) mosaic spread with a full width at half maximum (FWHM) of 25(5) minutes of arc. The plates shall be 1 mm thick and have lateral dimensions  $w \times h = 80 \text{ mm} \times 12 \text{ mm}$ . The plates shall be attached to the holder in sets of three and stacked with aluminum spacers to slightly offset the angles between them, so that the effective horizontal mosaic FWHM of the array is 60(6) minutes. Voids between the adjacent plates shall not exceed 0.5 mm.
- 3.3.2 **Heusler alloy monochromator:** An array of precisely aligned  $Cu_2MnAl$  crystals (well annealed so that the (111) Bragg reflectivity approaches that expected for ideally imperfect crystals) is to be mounted on a standard frame as described in section 3.1. The Mn moments in the crystals are to

be fully aligned by an external magnetic field produced by permanent magnets co-mounted with the frame. A polarization efficiency better than 95% and reflectivity better than 50% for polarized neutrons at a reference energy  $E_i = 15$  meV are defined as being acceptable. This monochromator assembly is to be procured from a vendor such as ILL or ORNL with a demonstrated ability to produce Heusler crystals of good performance.

- 3.3.3 **Optional additional monochromators:** A set of potassium-intercalated PG or synthetic mica crystals, whichever is more practical, is to be mounted on a standard GMI frame for very low-neutron-energy applications. Also to be considered as a possible future option is a high-wave-vector-resolution and/or perfect crystal focusing arrangement based on silicon or germanium crystals.

### 3.4 Monochromator exchanger

This device shall enable computer-controlled remote selection of one or the other of two crystal monochromator assemblies. Monochromator exchange is to take less than 1 minute. During typical operation exchange might occur as often as once a week. The exchanger should be designed so that either of the monochromators can be removed from the incident beam for service while the SNS is operating at full power.

### 3.5 Monochromator-to-sample supermirror guide

A vertically-tapered, vertically-converging supermirror guide, **G4**, with a supermirror coating of the largest practical critical angle larger than  $3\theta_c^{\text{Ni}}$  shall be located on the sample arm between the monochromator and sample. It should extend from as close to the monochromator as possible to within 400 mm of the sample. It shall be 40 mm wide; the inside height as a function of the distance,  $x$ , from the sample shall be given by

$$h(x) = h_s + \left( h_m - h_s \right) \frac{x}{L_{MS}},$$

where  $h_s = 40$  mm is the nominal sample height,  $h_m = 240$  mm is the monochromator height and  $L_{MS} = 1800$  mm is the nominal monochromator to sample distance. **G4** shall be split into three sections, **G4a**, **G4b**, and **G4c**, all mounted on the sample arm as described in section 3.1. A computer-controlled exchanger should permit remote replacement of the 150 mm long middle section **G4b** by a Fermi-chopper module as specified in section 3.6. Additionally there should be a computer-controlled exchanger permitting remote replacement of the 150 mm long **G4c** section (the closest to the sample) by one of a set of Soller collimators as specified in section 3.7. The guide sections shall be either evacuated or filled with  $^4\text{He}$  gas, wherever this will significantly reduce beam air scattering.

Each guide segment shall be centered and aligned with respect to a horizontal reference line connecting the sample rotation axis to the monochromator rotation axis. Centering should be accurate to within 0.5 mm and alignment accurate to better than 1 minute of arc. All guide segments inside the monochromator drum

are to be tightly embedded in the shielding. Materials that are illuminated by the monochromator and visible from the sample position should have the smallest possible incoherent scattering cross section.

### 3.6 Fermi-chopper

For high resolution applications, a computer-controlled exchanger shall replace guide section **G4b** with a module of matching size containing a Fermi-chopper, **T<sub>3</sub>**, designed to reduce the sample illumination times to  $10 \mu\text{s} < \tau_0 < 50 \mu\text{s}$ .

Because this chopper is not intended to be energy-selective it should have short, straight slots and rotate about a vertical axis in phase with the source at up to 480 Hz (8 times the source frequency). The outer diameter of the rotor shall be 120 mm or less, and the height of the slotted channel should match the exit height of the **G4a** section of guide.

### 3.7 Collimators

When necessary, a computer-controlled exchanger should make it possible to replace the guide section **G4c** nearest the sample with one of a set of four Soller collimators of identical external dimensions. The four collimators should define effective horizontal beam divergences of 20', 40', 60', and 120' respectively. Collimator blade thicknesses should be 0.1 mm or less. If feasible, the top and bottom surfaces of the collimators should have the same super-mirror coatings as guide **G4c**.

### 3.8 Monochromator shielding

The monochromator shall be surrounded by a neutron and gamma-ray absorbing composite shielding with a movable beam-port opening that is mechanically connected to the sample arm and rotates with it. To the extent practical it should be constructed of non-magnetic materials that have minimal long term neutron activation cross sections. The range of take-off angles accessible through the beam-port should be  $-5^\circ$  to  $120^\circ$ . It should take less than 2 min. to change the take-off angle from one extreme to the other. The combined monochromator crystal and beam-port rotation should define the monochromator crystal take-off angle to  $\pm 0.02^\circ$  or less. Whether the shielding mechanical design is to be based on a drum, pie-wedge section or other concept is yet to be determined.

The beam-port opening in the shield should be of internal dimensions that accommodate the converging guide **G4a-c**, the Fermi-chopper and the collimators. The shield design should also provide for incorporation of the remote exchange mechanisms. Shielding must be fitted tightly around all neutron optics elements attached to the sample arm as specified in sections 3.5-3.7 (with radiation steps where necessary) so that neutrons from the monochromator either pass through these elements or are absorbed in the shielding. The inner dimension of the shield should be such as to accommodate the monochromator crystal exchange mechanism with two monochromator crystal assemblies. Radiation protection requirements will determine the outer radius of the shield. It must contain neutron and gamma ray absorbing material sufficient to reduce the radiation rate and the background to acceptable levels: i.e. the radiation dose rate, and background outside the shielding and outside of monochromatic beam should



be no more than 5 mrem/hr at a distance 300 mm from the neutron beam and in compliance with all SNS radiation protection requirements and ALARA. Shield thickness should not exceed 1400 mm, so that a clearance of at least 400 mm between the shield and the sample axis is provided. Internal shield design should be such that the amount of the material inside the shield exposed to the incident neutron beam is minimized; all shielding around the monochromator that can be viewed from the sample position must be recessed in such a way that it is not directly illuminated by the incident neutron beam. A convenient access to the monochromators and other beam-line neutron optic elements for servicing and replacement must be provided.

The location and characteristics of the beam dump or “get lost” pipe (whichever is applicable) must be chosen to minimize its contribution to the detector count rate. In addition, an interlocked radiation exclusion zone around the instrument is to be defined in collaboration with the SNS operations staff.

### **3.9 Beam optics between collimator and sample**

A neutron optical bench shall be permanently attached to the sample arm and/or to the beam-port outside the shielding and aligned to better than 1 minute of arc with respect to a horizontal reference line connecting the sample rotation axis to the monochromator rotation axis as described in section 3.5. All components listed below are to be mounted on this bench downstream of the **G4** super-mirror guide. Components 3.9.1-3.9.3 shall be semi-permanently mounted; their combined thickness must not exceed 80 mm.

- 3.9.1 A beam monitor with a sensitive area larger than the exit aperture of the guide **G4c** and with a wavelength-proportional sensitivity that is no greater than  $10^{-5}$  at 15 meV.
- 3.9.2 A four position beam attenuator controlled from the main instrument control computer and capable of introducing three different planar objects into the beam. Two of the positions should provide 10 times and 100 times attenuation of the beam respectively at 15 meV. These two attenuators shall be permanently installed in the exchanger. The third position is to be slot that can hold a plate of width 40 mm, height 100 mm and between 1 mm and 10 mm thick. When selected by the attenuator exchanger this plate shall be positioned in the center of the beam to within 1 mm. The fourth position shall be a local beam shutter.
- 3.9.3 A computer-controlled, variable-opening, thermal neutron aperture covered with layer of LiF on the side facing the monochromator crystal. The aperture must be centered in the beam to within 0.5 mm and should have four independent degrees of freedom controlling the right, left, top and bottom opening with a positioning accuracy of better than 0.5 mm. The design should permit the width and height of the aperture to be varied from fully closed to the full width and height of the beam as defined by the exit aperture of the guide **G4c** as specified in section 3.5.

- 3.9.4 A computer-controlled aluminum flipper coil, not more than 20 mm thick, designed to rotate the neutron polarization in the incident beam by  $0^\circ$ - $180^\circ$ .
- 3.9.5 Auxiliary neutron optics components (of a total length not exceeding 150 mm) required for applications to be specified in the future.

## 4. Sample stage

The sample stage shall be rigidly attached to the sample arm and supported on the floor in such a way that it can move with the arm without tilting as it rotates to beam position defined by the monochromator crystal take-off angle. The positional accuracy of the sample stage should correspond to the same  $0.02^\circ$  precision as for the combined monochromator crystal and sample arm setting angle, as specified in section 3.8. Sample area shall be surrounded with interlocked shielding that reduces radiation levels to 5 mrem/hr or less and meets all SNS radiation protection requirements.

### 4.1 Space and location

The space available for sample stage positioning must allow monochromator crystal take-off angles covering the range  $-5^\circ < 2\theta < 120^\circ$ . Space for the power supplies, pumps and other auxiliary equipment required for both polarized beam operation and special sample environments must also be provided on the sample floor. The distance from the sample rotation axis to the monochromator crystal rotation axis shall be variable within restricted limits which are to be defined. It should be no greater than necessary to accommodate a Fermi-chopper, a Soller collimator, a neutron beam monitor, and polarized-beam equipment (such as a flipper) as specified in sections 3.5-3.9. A monochromator-to-sample distance  $L_{MS} = 1800$  mm is defined as nominal.

### 4.2 Degrees of freedom provided.

- 4.2.1 Sample rotation  $0$ - $360^\circ$  with an accuracy of 0.005 degrees.
- 4.2.2 Tilt of sample table  $\pm 12^\circ$  about two mutually perpendicular horizontal axes. Tilt accuracy must be better than  $0.1^\circ$  for loads in the range specified in section 4.3; the effective rotation axes must lie within 20 mm of beam center height.
- 4.2.3 Vertical translation of  $\pm 40$  mm above and below the beam center with positional accuracy better than 1 mm.
- 4.2.4 Horizontal translation of  $\pm 20$  mm along two mutually perpendicular horizontal directions parallel to the sample tilt axes, both with positional accuracy better than 0.5 mm.

### 4.3 Dimensions and load capacity.

The sample stage mounting surface shall be at least 152 mm below the beam center. Its on-axis load capacity shall be >500 kg. A (maximum) horizontal torque of  $5 \cdot 10^2 \text{ N}\cdot\text{m}$  should result in less than a  $0.1^\circ$  tilt of the sample rotation axis from the vertical.

#### **4.4 Materials requirement**

Sample table shall be made of non-magnetic materials. The force on any of its elements in a magnetic field gradient of 10 Gauss/mm should not exceed 1 N.

#### **4.5 Guide field**

A computer-controlled coils capable of generating either a vertical or a horizontal magnetic field larger than 10 Gauss throughout the neutron beam path around sample are to be provided. Coils should be mountable on the sample table and be large enough to accommodate a standard sample environment (ie provide a horizontal clearance of at least 400 mm in diameter around the sample axis).

### **5. Analyzer-Detector system**

#### **5.1 General principle**

Analysis of the scattered neutron energy will be by time-of-flight in a secondary flight-path of length  $L_{SD} = 4500 \pm 4 \text{ mm}$  as measured from the sample axis to the individual detector axis. The secondary flight-path shall include a variable vertical aperture after the sample, shielding, a gas-tight or vacuum-tight flight vessel containing either a radial collimator or a transmission polarizer assembly and a detector array as specified below. The secondary flight-path (analyzer) vessel shall be mobile, and designed to move on the floor in such a way that: (i) for all monochromator crystal take-off angles the axis of the cylindrical detector array remains vertical and coincides with the sample axis to an accuracy of better than 2 mm (ii) the detector bank can be sequentially moved (as specified by the experimenter) to those positions where the range of sample scattering angles accepted by detectors is best matched to the measurement.

#### **5.2 Detector bank**

The detector bank shall consist of a cylindrical array of identical, vertically mounted, one-dimensional, position-sensitive, tube-type  $^3\text{He}$  detectors centered on the sample axis and symmetric about the horizontal scattering plane. The angular size of the individual detector pixels (as seen from the sample position) shall not exceed 20 minutes of arc in either the vertical or horizontal direction. Each detector shall cover a scattering angle of at least  $\pm 7.5^\circ$  in the vertical direction; the horizontal angular coverage of the entire detector array will be at least  $60^\circ$ . Detectors shall have partial pressure of  $^3\text{He}$  gas and thickness to achieve 90% detection efficiency for 15 meV neutrons.

An array of 190 or more 64-pixel, position-sensitive detectors 20 mm to 25 mm in diameter and 1200 mm to 1300 mm long satisfying the above specifications are to be purchased from an established detector manufacturer. They shall be mounted

with their axes vertical to within 5 minutes of arc and positioned with an accuracy of 2 mm on a 4500 mm radius circle in the horizontal plane. This is also the accuracy to which the detectors are to be co-centered at the nominal beam-sample height. Voids between adjacent detector tubes are not to exceed 1 mm.

The detector array shall be fixed inside the mobile analyzer vessel. The vessel design will allow the detector array rotation around an axis concentric with the sample axis to within 2 mm with the accuracy of angular positioning better than  $0.02^\circ$ . Detector voltage supplies, preamplifiers and primary acquisition electronics shall be mounted on the analyzer vessel and move with it to reduce the number of cables connecting the mobile detector array to the stationary part of the data acquisition system to 1 or 2 high-speed, optical or other, communication lines.

### 5.3 Analyzer vessel

Except for the initial 400 mm downstream of the sample axis, the path of the neutrons scattered by the sample shall be contained within a mobile secondary flight-path (analyzer) vessel which is to be either evacuated or  $^4\text{He}/\text{Ar}$  gas-filled, to minimize beam loss and background from air scattering. The auxiliary equipment needed to either maintain vacuum or gas pressure shall be permanently mounted on the vessel and shall move with it. Either a radial collimator or a transmission polarization analysis assembly shall be positioned in the scattered beam inside the flight vessel, with its upstream face at a nominal distance of 400 mm from the sample axis, as specified in sections 5.6-5.7. The vessel shall be equipped with a computer-controlled automated exchanger that selects either one of the four radial collimators or one of the two polarization analysis assemblies.

5.3.1 **Materials:** The analyzer vessel shall be made of high-strength aluminum alloy or similar non-magnetic material with a low neutron activation cross section. Its inner walls and all parts of the collimator or polarization analysis assembly that are visible to the detector array should be covered with a neutron-absorbing material such as  $\text{B}_4\text{C}$  or  $\text{LiF}$ . The scattered beam entrance window on its upstream face should be made of high neutron transparency, high strength aluminum alloy and be of the minimal thickness necessary to support either vacuum or a small over-pressure of gas within the vessel.

5.3.2 **Dimensions:** The size and the shape of the inner and outer cylindrical walls of the flight vessel shall be designed to (i) allow either a one of the radial collimators or one of the polarization analysis assemblies be positioned with its upstream face 400 mm from the sample; (ii) provide space for the automatic exchanger and the collimators and polarization analysis assemblies that are not in use, and (iii) accommodate the detector array which is to be rigidly attached the vessel to the vessel outer wall inside. A removable port(s) are to be provided for convenient access to the automatic exchanger and the detector array. The flat walls on the sides, top and bottom of the vessel are to have inner dimensions which restrict the area of sample illumination to the size of the detector array. For example,

the inner height,  $h(x)$ , of the vessel should vary with distance,  $x$ , from the sample axis in accord with the expression

$$h(x) = h_s + (h_d - h_s) \frac{x}{L_{SD}},$$

where  $h_s=40$  mm is the nominal sample height,  $h_d= 1280$  mm the nominal detector height and  $L_{SD} = 4500$  mm the sample to detector distance.

- 5.3.3 **Position:** The analyzer vessel shall move on the floor following the sample arm so that the axis of the cylindrical detector array coincides with the sample axis with a positioning accuracy of better than 2 mm, as described in section 5.1. The accuracy of the detector bank angular positioning with respect to the axis of the beam incident on the sample should be better than  $0.02^\circ$  and should be reproducible after 1000 analyzer vessel movements. If not restricted by the incident guide and associated shielding, sample scattering angle extreme positions of  $-5^\circ$  and  $+120^\circ$  should be accessible to at least one detector for all monochromator take-off angles. It should take less than 2 minutes to move the analyzer vessel with detector bank between the extreme angular positions. Vessel support and moving systems shall be chosen to minimize the cost of construction, operation and maintenance while at the same time meeting all of the above-listed specifications.

#### 5.4 Variable vertical aperture after sample

Upstream of the secondary flight-path shielding (but as close to the sample as practical) there shall be a computer-controlled slit capable of restricting the height of the beam scattered by the sample from  $h_{\min}= 0$  mm to  $h_{\max}= 100$  mm. This slit should be centered to within 1 mm of the beam-center height and have top and bottom apertures that are independently motorized and controlled. It can either be an independently mounted device made of 40 mm thick  $B_4C$ -rich material and covered with LiF on the side facing the sample or a mobile extension of the analyzer shielding that can be positioned as close to the sample as needed.

#### 5.5 Shielding

Shielding made of high neutron cross-section materials shall be placed around the analyzer vessel. This shielding shall either be a stationary structure enclosing all possible analyzer positions or be attached to the mobile analyzer vessel itself; the choice is to be made on the basis of practicality and cost-efficiency. In either case, the shielding inner surface shall be covered with a thermal-neutron-absorbing material such as cadmium or LiF. A background count rate of 1 count/min/detector when the SNS is operating but both the beamline shutter and the shielding entrance window are closed is defined as being acceptable. The interior height of the stationary shielding must be sufficient to contain the analyzer vessel and all auxiliary equipment mounted on it, as specified in section 5.3. Also, its top must be modular and allow for easy access to the analyzer vessel for maintenance and, if necessary, replacement of the vessel and/or its

components. If MCNP-X neutronics calculations establish the necessity of a “get-lost” pipe, it should be incorporated into the shield design.

5.5.1 **Dimensions and position:** The shielding should start as close as possible to the variable vertical aperture after the sample specified in 5.4. The distance from the sample axis to the upstream face of the shielding shall be such that the analyzer vessel can be positioned with the upstream face of the radial collimator or polarization analysis assembly (whichever is in place) 400 mm from the sample axis. This shielding should have a 100 mm tall scattered beam entrance window and a computer-controlled horizontal aperture of width and position that can be varied so that a selected number of detectors (from a minimum of 1 to a maximum of all detectors in the array) are visible from the sample position. It should be so designed that - if not restricted by the incident guide and its associated shielding - extreme sample scattering angles of  $-5^\circ$  and  $+120^\circ$  are accessible to at least one detector at all monochromator take-off angles as specified in section 5.3.3. A sufficient clearance downstream the flight vessel should be provided to permit easy assembly and maintenance of the detectors and detector electronics.

5.5.2 **Beam stop:** In some positions of the analyzer vessel the axis of the primary beam could intersect the detector array. It will therefore be necessary to have either a primary beam stop or a “get-lost” pipe to prevent the primary beam from either directly impinging on the detector array or creating an unacceptable background of primary beam neutrons scattered into the detector array. A beam stop should be designed to produce as little neutron and hard gamma radiation as possible; its exterior width should be minimized and its position chosen so that it cannot scatter neutrons into any of the active detection channels.

## 5.6 Radial collimators after sample

Immediately behind the upstream face of the analyzer vessel there shall be a four-position collimator exchanger capable of accurately positioning any one of four radial collimators or, alternatively, one of two polarization analyzer assemblies in the scattered beam. In all positions the collimator axes should be concentric with the sample axis to better than 2 mm. Changes from one collimator or polarization analyzer to another are to be effectuated from a control computer and should take less than 30 seconds. All collimators are to be embedded in high boron content neutron shielding material in such a way that neutrons either pass through the window of the collimator or are absorbed. In addition, the lateral dimensions of their entrance windows should match the lateral dimensions of the entrance window of the flight vessel and their internal dimensions should match the dimensions of the scattered beam illuminating the detectors in the same way as the inside surfaces of the analyzer vessel match the scattered beam dimensions, as specified in section 5.3.2. The spacing between blades is to be determined by the expression

$$d = \alpha \ell ,$$

where  $\ell = 200$  mm is the length of the collimator blades and  $\alpha$  is the effective beam divergence. Horizontal divergence angles  $\alpha$  for the four collimators shall be 20', 40', 60' and 120' respectively. Blade thicknesses should be 0.1 mm or less.

All the radial collimators are to be positioned with the sample rotation axis as their focal point to within 2 mm and should be parallel to one another to within 0.01 degree. A line passing through the central blades of the collimators should also pass through the sample rotation axis to within 2 mm.

### **5.7 Broadband transmission polarizers.**

It shall be possible to place either of two broadband, multi-channel supermirror transmission polarization analysis assemblies in the same position as the radial collimators (i.e. immediately behind the upstream wall of the analyzer vessel, at 400 mm from the sample axis) using the same computer-controlled collimator exchange mechanism. One of the two polarization analysis assemblies is to be configured for optimum performance at 15 meV; the other at 7.5 meV. It should also be possible to substitute the polarization analysis assemblies for radial collimators in the exchanger. Changing from one combination of polarization analyzers and collimators to another will be done manually and should not take more than 30 minutes to complete. Like the collimators, the polarization analyzers are to be embedded in a boron-rich neutron shielding material so that neutrons either pass through the polarizing windows or are absorbed.

**5.7.1 Polarization analysis assembly:** Each polarization analysis assembly is to consist of 19 identical channels mounted in a common magnetic frame supplying a permanent magnetic field of at least 300 Gauss; i.e. a field sufficient to magnetically saturate the polarization-sensitive supermirror coatings in all channels. Each channel is to be 20 mm in over-all width and have a height profile that matches the scattered beam height as specified in section 5.3.2. The height should not, however, exceed  $200 \pm 10$  mm at its downstream end. The channels should be equally spaced on the circumference of a circle centered at the sample position with an accuracy of 2 mm, and co-leveled with the sample height with the same accuracy. Tight fitting, wedge-shaped neutron absorbing spacers are to be placed between channels to assure that all neutrons incident on the detectors pass through and not between the channels. Sample scattered neutrons passing through the channels will be split into two separate beams of opposite polarization. The channels should be designed so that the oppositely polarized beams from each channel are fully separated at the detector position but are not overlapped by beams from adjacent channels for scattered neutron energies  $3 < E_f < 30$  meV.

**5.7.2 Individual polarization analysis channel:** Each channel shall consist of a 20 mm wide and 150 mm long collimator immediately followed by a stack of 20 mm wide, polarization-sensitive, supermirror-coated, thin silicon wafers 50 mm long and tall enough to accept the full scattered beam height as specified in section 5.7. Aluminum spacers are to be used to bend the silicon wafer stacks to a horizontal cylindrical curvature that

optimizes the polarization analysis efficiency of the channel at the nominal neutron energy for which it is designed. The collimator and polarization analyzer are to be placed in a rigid frame and co-aligned so as to achieve optimum beam transmission and polarization analysis efficiency at the nominal neutron energy. A choice of 10', 20' or 40' collimation should be provided for each channel. The critical angle of the supermirror coating for one neutron polarization direction should be at least  $3\theta_c^{\text{Ni}}$  (or larger if possible) and for the other it should be no larger than  $\theta_c^{\text{Ni}}$  (or smaller if possible). Over-all, the transmission of the polarized collimated beam through the channel is to be better than 90% for energies  $3 < E_f < 30$  meV. The center-line of every polarization analyzer collimator should pass through the sample rotation axis to within 2 mm.

## 6. Instrument Control and Data Acquisition

Three independent computer systems are to be supplied with the instrument. To the extent possible, standard software developed by the SNS staff is to be utilized.

**6.1 Instrument Control System.** An Instrument Control Program (ICP) running on a dedicated computer shall control the status and operation of all instrument systems as specified in this document, including any automated sample environments needed for particular measurements. The ICP shall communicate with the data acquisition program (section 6.2) to provide information about the instrument configuration and to synchronize and up-date their mutual status during the course of the experiment. The ICP shall also communicate with the experiment planning and data analysis program (section 6.3) to make it possible for the experimenter to pre-select optimum instrument configurations and input parameters for the planned measurement.

**6.2 Data Acquisition System (DAS).** There shall be a separate, dedicated computer with an advanced high-capacity storage system that is able to communicate with the detector electronics and collect, pre-process and store the data from the individual detectors. Data is to be stored in files using the HDF-type (hierarchical data) format common to all SNS instruments. Along with the data, the files should contain headers with a complete description of the instrument configuration and instrument parameters provided by the ICP.

**6.3 Experiment Planning and Data Analysis Program (EPDAP).** HYSPEC shall have a dedicated and integrated software package, EPDAP, to plan measurements so as to take optimal advantage of the wide-angle, multi-channel TOF analyzing system and also to analyze the data. The EPDAP should run on a separate, dedicated computer equipped with an extensive set of the peripheral devices for data transfer and visualization. It should be able to communicate with the ICP to export/import the instrument parameters and with the DAS to read the data for analysis and visualization.

## 7. System Wide Requirements



**7.1 Hard and soft limits.** All instrument degrees of freedom must be equipped with soft and/or hardware limits that prevent collisions but allow a full range of physically achievable positions. Sample rotation is a special case where hardware limits must be variable to allow for the different constraints imposed by different sample environments.

**7.2 Automated calibration and alignment.** There should be an automated detector calibration procedure and an automated alignment protocol for all degrees of freedom of the instrument.

**7.3 Permanent electrical wiring.** The number of cables should be minimized; wherever possible optical communication lines are to be used. All wiring is to be permanently installed and is to comply with all applicable industry and SNS standards.

**7.4 Crane.** There must be an overhead crane capable of lifting weights of more than 1 metric ton such as, for example, major secondary flight-path instrument components. It should also be capable of lifting heavy (and more than 1500 mm tall) sample environment devices - such as, for example, cryomagnets - and mounting them on the sample table. Crane coverage should extend over the monochromator shielding, the sample table and the secondary flight-path systems.

**7.5 Radiation Safety Exclusion zone.** In accordance with the “as low as reasonably achievable” radiation safety requirements, the instrument is to be surrounded by an interlocked exclusion zone within which personnel will not be permitted when the primary shutter is open and the beam is on. Details are to be specified by SNS Health Physics.

(1) Metric units have been used throughout this document. Where standard stock sizes of materials differ from those specified, the closest four-digit decimal inch value is to apply.

## Appendix D. HYSPEC Estimated Budget and Funding Profile

ITEM	Direct cost in FY03 \$	Burden Allowance @10%	Contingency Factor	Contingency	TOTAL w/ Burden & Conting.	Esc to At Year \$ FY03	Esc to At Year \$ FY04	Esc to At Year \$ FY05	Esc to At Year \$ FY06	Esc to At Year \$ FY07	Esc to At Year \$ FY08	At Year Total
<b>Technical Construction</b>												
<b>Primary Flight Path</b>												
T0 chopper	218	22	25%	60	300	-	-	316	-	-	-	316
Frame overlap chopper	131	13	25%	36	180	-	-	190	-	-	-	190
Counter-rotating disk choppers	364	36	25%	100	500	-	-	527	-	-	-	527
Fermi chopper	364	36	25%	100	500	-	-	527	-	-	-	527
Steel jacketed m=3 guides	291	29	25%	80	400	-	-	-	434	-	-	434
Shutter insert m=3 guide	131	13	25%	36	180	-	-	-	195	-	-	195
Guide shielding	873	87	25%	240	1,200	-	-	-	1,301	-	-	1,301
Beam monitors	29	3	25%	8	40	-	-	42	-	-	-	42
Sub total	2,400	240		660	3,300	-	-	-	-	-	-	3,533
<b>Monochromator Section</b>												
Monochromator	-	-	-	-	-	-	-	-	-	-	-	-
Drum Shield	945	95	25%	260	1,300	-	-	-	1,410	-	-	1,410
Crystals and holders	182	18	25%	50	250	-	-	264	-	-	-	264
Tapered m=3 guide	73	7	25%	20	100	-	-	-	108	-	-	108
Collimators	36	4	25%	10	50	-	-	53	-	-	-	53
Beam monitor and slits	44	4	25%	12	60	-	-	63	-	-	-	63
Shielded get-lost pipe	436	44	25%	120	600	-	-	-	651	-	-	651
Beam stop	145	15	25%	40	200	-	-	-	217	-	-	217
Sub total	1,862	186		512	2,560	-	-	-	-	-	-	2,765
<b>Sample Stage</b>												
Goniometer and support	109	11	25%	30	150	-	-	158	-	-	-	158
Removable shielding	73	7	25%	20	100	-	-	-	108	-	-	108
Ancillary equipment	76	8	20%	17	100	-	-	-	-	111	-	111
Sub total	258	26		67	350	-	-	-	-	-	-	378
<b>Detector System</b>												
190 position-sensitive detectors	415	41	25%	114	570	-	-	601	-	-	-	601
Detector support structure	44	4	25%	12	60	-	-	-	65	-	-	65
Collimators/positioner	145	15	25%	40	200	-	-	-	217	-	-	217
19 Polarization analyzers	582	58	25%	160	800	-	-	-	867	-	-	867
Rotating Detector vessel	582	58	25%	160	800	-	-	-	867	-	-	867
Beam controls-DAQ	80	8	25%	22	110	-	-	116	-	-	-	116
Detector shield	655	65	25%	180	900	-	-	-	976	-	-	976
Sub total	2,502	250		688	3,440	-	-	-	-	-	-	3,710
<b>Data Collection System</b>												
Mezzanine	45	5	20%	10	60	-	-	-	-	-	68	68
Control cabin	30	3	20%	7	40	-	-	-	-	-	46	46
Furnishings	8	1	20%	2	10	-	-	-	-	-	11	11
Miscellaneous	29	3	25%	8	40	-	-	-	11	11	23	45

R&D; choppers/polarizers	182	18	25%	50	250	-	256	-	-	-	-	256
Sub total	294	29		76	400	-	-	-	-	-	-	426
<b>CAPITAL TOTAL</b>	<b>7,315</b>	<b>732</b>	<b>25%</b>	<b>2,003</b>	<b>10,050</b>	-	256	2,858	7,427	122	148	<b>10,812</b>
<b>Labor</b>	-	-		-	-	-	-	-	-	-	-	-
Installation technicians	1,061	106	20%	233	1,400	-	-	-	-	445	1,140	1,585
<b>LABOR TOAL</b>	<b>1,061</b>	<b>106</b>	<b>0</b>	<b>233</b>	<b>1,400</b>	-	-	-	-	445	1,140	<b>1,585</b>
<b>Technical Construction Total</b>	<b>8,376</b>	<b>838</b>	<b>0</b>	<b>2,236</b>	<b>11,450</b>	-	256	2,858	7,427	567	1,288	<b>12,398</b>
<b>Project Management &amp; Engineering</b>	-	-		-	-	-	-	-	-	-	-	-
Project Management	661	66	10%	73	800	-	164	169	173	178	182	867
Project Engineer/Scientist	661	66	10%	73	800	80	246	169	173	178	-	846
Designer/Engineer ORNL shielding studies	579	58	10%	64	700	50	205	211	217	56	-	738
ORNL support/liason	207	21	10%	23	250	250	-	-	-	-	-	250
Software	103	10	10%	11	125	-	-	-	-	-	143	143
Travel	227	23	20%	50	300	-	-	79	81	83	86	329
Proj. Mgt & Engrg. Total	269	27	10%	30	325	25	62	63	65	67	68	350
<b>Proj. Mgt &amp; Engrg. Total</b>	<b>2,700</b>	<b>300</b>	<b>10%</b>	<b>300</b>	<b>3,300</b>	380	615	628	645	940	1,551	<b>4,758</b>
						-	-	-	-	-	-	-
<b>Project TEC</b>	<b>11,076</b>	<b>1,138</b>		<b>2,536</b>	<b>14,750</b>	<b>380</b>	<b>871</b>	<b>3,486</b>	<b>8,072</b>	<b>1,507</b>	<b>2,839</b>	<b>17,156</b>
<b>Other Costs</b>												
Program Development	826	83	10%	91	1,000	-	205	211	217	222	228	1,083
<b>OTHER TOTAL</b>	<b>826</b>	<b>83</b>		<b>91</b>	<b>1,000</b>	-	<b>205</b>	<b>211</b>	<b>217</b>	<b>222</b>	<b>228</b>	<b>1,083</b>
<b>Total Project Cost (TPC)</b>					<b>15,750</b>							<b>18,239</b>