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Zeemans: A High Magnetic Field Beamline for the SNS

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ABSTRACT

Neutron scattering experiments and bulk experiments in high magnetic fields have been principal means of investigating properties of materials on scales ranging from Angstroms to micrometers. The Zeemans instrument, proposed to be built at SNS will combine these tools and thus lead new scientific discoveries. Some of the possible research avenues that will benefit from higher magnetic fields are the study of correlated electronic systems and quantum magnetism, structural phase diagrams of magnetic alloys, or the configuration of hydrogen storage materials. A shielded 25 - 30 T superconducting magnet, using YBCO tape technology for the inner coils and Cable-In-Conduit Conductor for the outer coils, is under development at the National High Magnetic Field Laboratory for installation on Zeemans. Such a magnet provides an order of magnitude increase in electromagnetic energy density compared to other neutron scattering capable magnets in the United States. The size of the magnet and the required connections to utilities means that its position should be fixed and an instrument that is capable of performing all of the scattering methods designed around it. Zeemans will be able to operate in the following modes: neutron diffraction (powder and single crystal), SANS, reflectometry, and spectrometry. The unique features, such as the guide, chopper, changeable optics and rotating scattering chamber designs, that allow these multiple modes of operation and stay within the constraints of existing SNS facilities, will be discussed in this contribution.

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1. Introduction

To maximize the science that can be performed with the high field magnet, Zeemans is designed to be configurable to allow multiple modes of operation. While traditionally provided by distinct instruments the unique thermodynamic conditions, offered by the ZEEMANS magnet, call for a high degree of versatility. This study covers such a design. It demonstrated that a neutron instrument capable of doing, single crystal diffraction, direct geometry neutron spectroscopy, powder diffraction, Small Angle Neutron scattering, and neutron reflectometry can be built around the magnet.

The instrument will be located on the Coupled H_2 moderator as viewed by beamline 14 A at the Spallation Neutron Source at Oak Ridge National Laboratory. This moderator provides the highest flux of neutrons with energy scales well matched to the magnetic field provided by the magnet and with numerous scientifically relevant systems.

A description of the instrument is provided below. A novel guide system transports the neutrons 70 m to the sample position located in the center of the magnet. This guide design provides maximum flux at the sample position within the constraints given by neighboring beamlines and the existing building configuration. A series of bandwidth choppers are used to avoid frame overlap for all modes of operation and high speed choppers are included to provide the sharp time pulses necessary for spectrometry. These high speed choppers would be stopped in the open position for wide bandwidth modes of operation. An additional high speed chopper will be located, near the frame overlap choppers, to limit sub frame overlap from the sub frames in the repetition rate multiplication mode (RRM) of operation. The neutrons scatter off of a sample that is as large as 2cm x 2cm in cross section, and out through the horizontal cones of the magnet in both the forward and backward directions to linear position sensitive ^{3}He detectors located 5 m from the sample position. A 3 dimensional CAD view of the full Zeemans beamline is shown in Figure 1.

Figure 1. CAD model of the ZEEMANS instrument. Showing (From the left to the right), The neutron guide, the 4 bandwidth choppers, two high-speed choppers the backward scattering detector bank, the magnet on the rotation stage and the forward scattering detector bank.

Immediately upstream of, and up to 5 m before, the sample position is a section of interchangeable optics. These optic elements allow optimization of the incident beam characteristics for specific sample and measurement types. For example if the sample is large, a weak scatterer, and fine momentum transfer (**Q**) resolution is not critical, focusing optics will provide maximum flux on sample. Alternatively for SANS type measurements, where fine **Q** resolution is critical, an aperture can be automatically inserted at the 5 m position.

The ability to use polarized neutrons with high magnetic fields on ZEEMANS provides key scientific opportunities including the ability to resolve hydrogen locations in complex structures and probing the anisotropy and chirality of magnetic structures and fluctuations. Towards this end, an incident beam wide band polarizer will be located near the high speed choppers and the detector tank will include a supermirror analyzer for polarization analysis. The analyzer can be removed for non-polarized operations.

2. *Incident flight path*

After the moderator a state of the art neutron guide will transport neutrons from the moderator to the sample position. The design of the guide curves, in the horizontal direction, to remove line of sight between the moderator and the sample and to avoid a target building structural column. A compact beam bender will be used to curve the beam over a short distance.

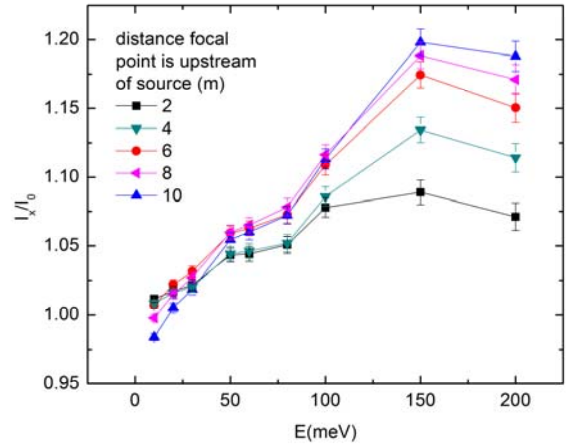

Figure 2. The intensity gained by opening the front end of the guide. The opening is increased by starting the guide at the same position, but shifting the position of the focal point up stream by the amount described on the plot.

In the vertical direction, the guide will use elliptical focusing with the upstream focal point behind the moderator to capture more flux and the other focal point at the sample position. Monte Carlo Ray tracing with McSTAS[1-2] was performed to determine the optimal upstream position. The guide was constrained to be 15 cm tall and start 2 m away from the moderator.

Figure 2 shows the comparison of several different possible configurations. In each configuration the guide starts at the same position and the opening is controlled by the placement of the upstream focal point. The 6m position is chosen as an optimum over the full wavelength range. For the purposes of optimizing the shape, the guide index was fixed at m = 3.6.

The portion of the guide closest to the sample will be changeable to allow control of divergence on the sample and to provide polarization capability. The focusing capabilities are provided by the elliptical guide. Slits will be used to provide collimation when a less divergent or pinhole geometry is required. One horizontal and one vertical pair of slits will be placed at the entrance of the vacuum vessel; 5 meters before the sample. The polarizing capabilities include a polarizing guide for long wavelengths, a ^{3}He cell for higher incident energies, polarizer, and a spin flipper.

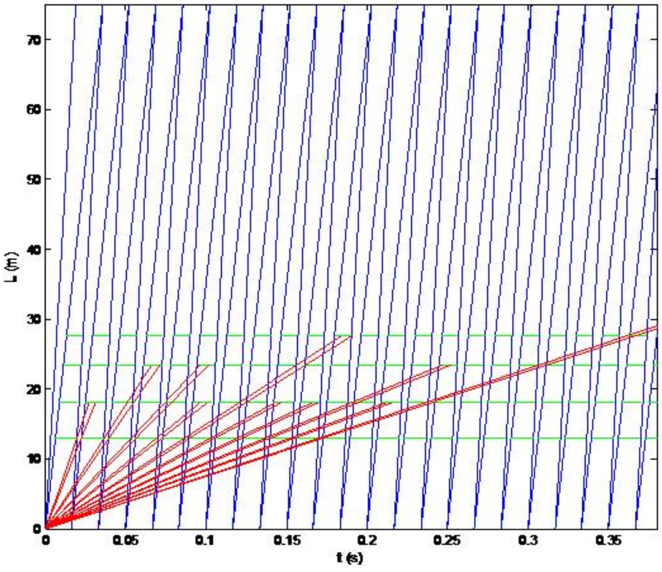

Figure 3. The timing diagram showing that only the desired neutrons with wavelengths less than 37 angstroms are transmitted

3. Frame Overlap choppers

Frame overlap choppers isolate the time-frames of neutrons incident on the detectors from each other. For white beam instrument operation, one wants to maximize the bandwidth through the instrument and then use choppers to ensure that the wavelength at which frame overlap occurs is sufficiently long that an insignificant number of these neutrons is generated from the source. The minimum number of choppers that can be used for this purpose is three. However, this number increases if there is a limitation on how close to the moderator that the first chopper can be located. In the case of Zeemans the first chopper can be placed no closer than 13 m from the moderator due to HySpec on beamline 14B. With the first chopper placed at 13 m, a timing diagram in Figure 3 shows that four frame overlap choppers are necessary to limit frame overlap to wavelengths > 37 Å. In addition these choppers can be phased to transmit only every other source pulse and thus double the frame for the SANS and reflectometry modes of operation.

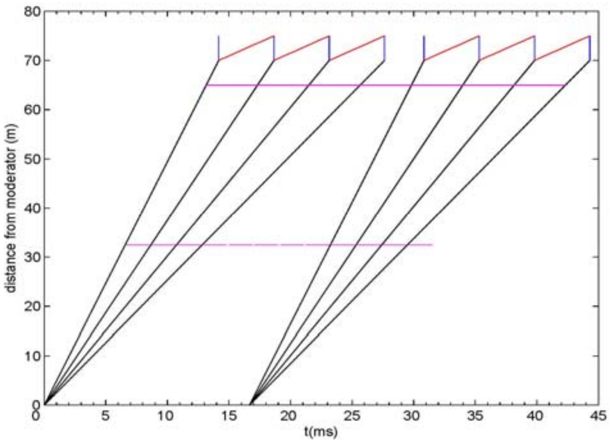

Figure 4 The timing diagram for spectroscopy mode using 4 RRM pulses. Pink lines show choppers 5m from the sample and an additional chopper at 32 m to separate the RRM frames

4. High speed choppers

High speed choppers will be employed 5 m upstream of the sample position to enable the spectroscopy mode. These choppers are envisioned as high speed double disc as they are the most flexible in the cold to thermal energy range, for which this instrument is designed. A cutout the width of the guide is ~ 3.8 cm wide. For double disc choppers, counter rotating at a speed of 300 Hz a-piece, this opening will provide a 52 µs pulse. A narrower cutout of 1 cm width could also be included to provide a high resolution mode. This configuration would provide a 13.6 µs pulse. The resultant resolution for these conditions will be discussed later.

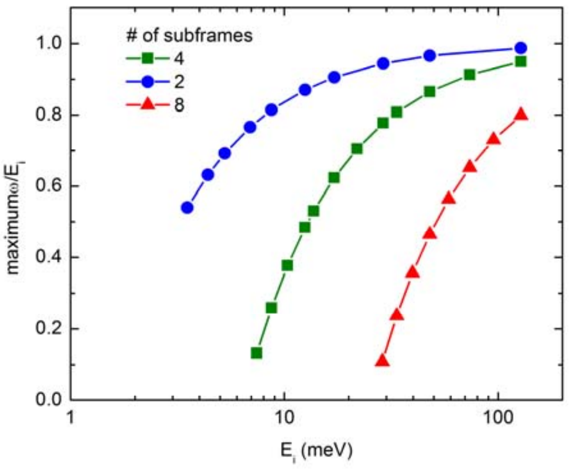

Figure 5. The ratio of the maximum energy transfer to incident energy before frame overlap for different numbers of sub frames per frame

A novel way to increase the speed of data collection is to use a technique called Repetition Rate Multiplication (RRM)[3-4]. The idea is to cut the source pulse multiple times thus putting multiple wavelengths on the sample in a single measurement. An example for 4 pulses is shown in Figure 4. An additional chopper, which runs at 240 Hz, must be located at ~ 32 m to remove cross talk between frame RRM pulses.

The limit of this technique is determined by how much frame overlap one can tolerate and still obtain usable data. The case shown in Figure 4 is a relatively conservative estimate. Figure 5 shows that overlap can be avoided in cases with less than 4 sub frames. Recent work by Russina and Mezei [4] shows in certain cases an aggressive analysis approach can be used to deconvolve a signal from significantly overlapping frames. Nevertheless, with a flexible set of disc choppers, that choice can be decided for each experiment

5. Vacuum Vessel

The vacuum vessel serves multiple purposes. It provides an evacuated flight path for background reduction and thermal isolation for sample environments, and its shielding provides a low background environment for the detector bank. Furthermore it will be made from non-magnetic material to reduce interference with the magnet. The vacuum chamber will be ~ $18m^3$ of volume and, will be evacuated to $1x10^{-6}$ Torr. A rotary seal on the top and on the bottom (see Figure 6) provides the interface between the scattered beam portion of the chamber and the magnet interface. This allows the magnet to rotate while the detector portions of the chamber remain stationary. Each seal is ~ 2m in diameter and does not exceed the scalability of standard differentially pumped designs. The magnet is connected to the vessel with standard vacuum flange seals and a bellows to accommodate design tolerances. These flanges facilitate quick removal of the magnet for maintenance. Concepts where the whole vacuum chamber moves or the whole magnet was in vacuum were considered but abandoned because preserving the alignment of the optics or so closely integrating the magnet and the instrument are greater engineering challenge that the aforementioned seals.

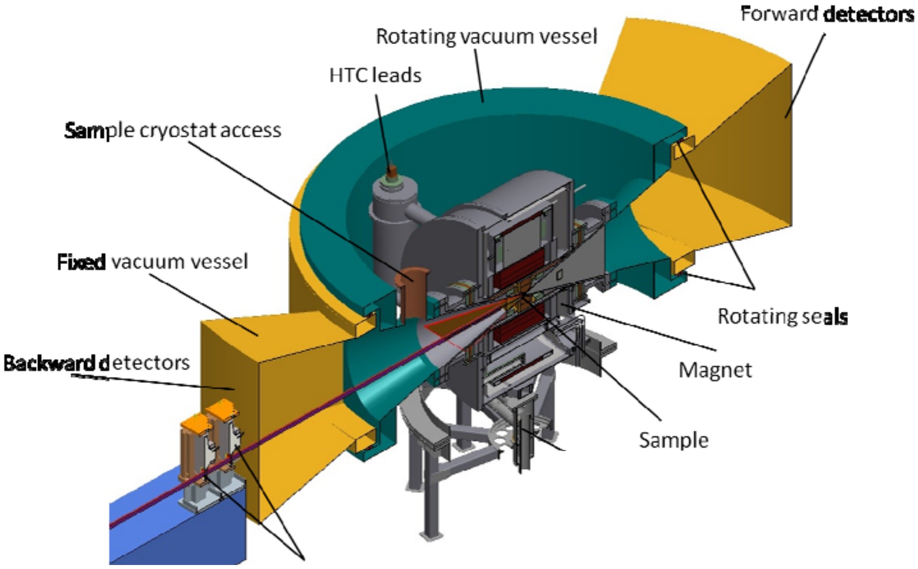

Figure 6 Cross section of the secondary flight path showing the major components.

The inner rotating portion further contains the interface to the sample environment equipment.

6. Detectors

Linear Position Sensitive detectors (LPSDs), where He^3 is the detection gas are planned for Zeemans. These detectors will be 7 mm in diameter and placed at a distance 5 m from sample position; both in the upstream and downstream detector position. The angle coverage of the detector array will fully cover the cone angle and in addition will cover the additional area needed when the magnet is rotated 15°. The detectors and their electronics will be in the vacuum space. The 5 meter final flight path was chosen by the desired energy resolution for spectroscopy. Figure shows the resolution as a function of final flight path length and various parameters that control the cost of the final flight path. Beyond 5 meters there is little gain in resolution for a significant increase in detector area, vessel surface area, and vessel volume. The detector width was chosen to achieve adequate angular resolution for SANS.

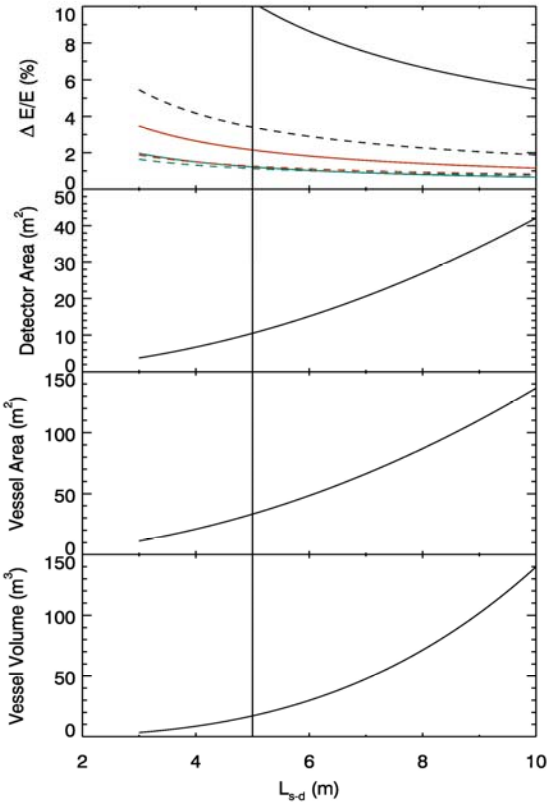

Figure 7. The instrument resolution vs. the length of the secondary flight path, as compared to several scaling parameters for sizing the detector vessel.

7. Sample environment

Control of the sample temperature and orientation is essential to the scientific program. The ability to rapidly load and exchange samples will allow the most efficient data collection. The magnet configuration requires that the sample is loaded, and cryogenic services supplied, horizontally. A solution to these complications is summarized below and in Figure . The magnet vacuum space will be independent of the sample space and will accommodate a 20 mm x 20 mm sample and the necessary rotation mechanism.

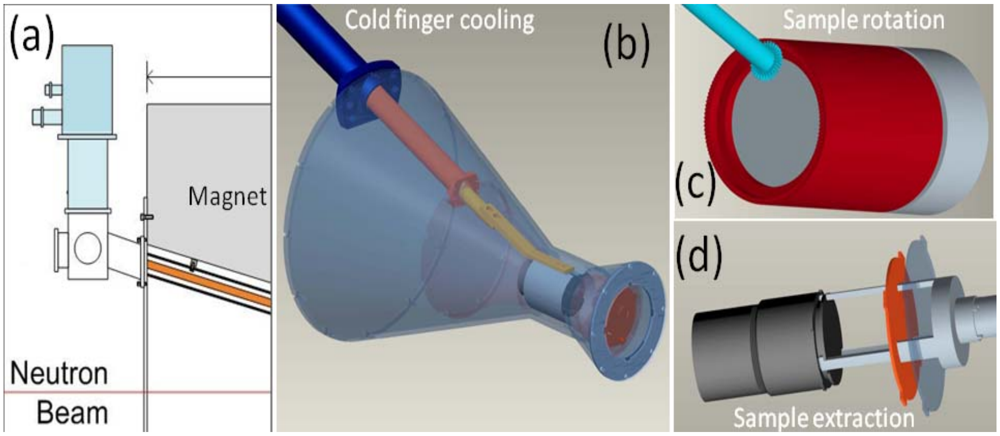

Figure 8. (a) Cryo-port linking cryostat to cold finger. (b) Cold finger enters high field region. (c) Concept for sample rotation about field axis. (d) Fixture for cold sample extraction from opposite end of magnet. Shown are sample cell, extraction tool, and heat shields that are extracted with sample.

All temperature control will come down the upstream bore. A long cold finger is envisioned for heat removal Figure 8(b). This will attach to standard sample environment equipment on the upstream side Figure 8 (a). The thermal gradient over a 2 m long Cu cold finger, with a actively cooled 50 K heat shield, was studied by finite element analysis. The results showed a 2 K temperature difference across it. Therefore a standard 4 K cryocooler stationed upstream should cool a sample to about 6 K. With additional heat shields and actively cooled cold fingers (e.g. add JT stage) one can expect 2 K on sample, and horizontal dilution refrigerators are the route to mK The cold finger will be changed out with a specialized furnace for high temperature operation.

Rotating the sample around the field direction is crucial as it provides access to **Q** space for single crystal samples. To do this, the upstream side of the sample cell will have teeth that mesh with a gear that remains in place. The rotation will likely be activated via a piezo motor so it can be cooled and thus minimize heat leaks. A view of the concept is shown in Figure 8 (c)

To change samples, the magnet will be rotated beyond the detector array to a load lock. This loading chamber will be equipped with a remote handling tool to grab the sample can and the heat shields. This tool will allow the sample can to be inserted with the heat shields and then the tool will be removed before the start of the measurement. This mechanism will expedite sample changes while preserving the vacuum.

8. Magnet

The ZEEMANS magnet is designed to produce a field of 25-30 T on axis using all superconducting coils. The magnet warm bore is defined by a central cylindrical region of 50 mm diameter and 62 mm length, which opens into a conical shape toward both ends with a cone-angle of 15 degrees from the central axis. The magnet consists of a Nb_3Sn CICC (cable-in-conduit conductor) [5-6] outer magnet giving a field of 13 T, and an adiabatically stable inner magnet containing four YBCO and one Nb_3Sn coils giving a field of 12-17 T as shown in Figure 9. The magnet is shielded to cancel the dipole moment using separate shield coils for the inner and outer magnets. The outer magnet shield coil is a CICC coil using Nb-Ti conductor, while the inner magnet shield coil is wound over the outer magnet shield coil as a single layer of Nb-Ti wire. The field uniformity of the combined magnet is better than 0.2 % in a central region of diameter 20 mm and length 20 mm. The outer magnet and shield coil operate in series at 20 kA. The inner magnet and series shield coil operate below 200 A. The stored energy of the magnet is 50 MJ, with a self-stored energy of 2.6 MJ for the inner magnet, 39.4 MJ for the outer magnet, and 8 MJ of mutual energy. The magnet is contained in a horizontal warm bore cryostat shown in Figure 9. In addition, the cryostat is mounted on a rotation stage to allow 15° magnet rotation for scattering angles up to 30°. By building ZEEMANS in an all-superconducting configuration, the magnitude of required power, chilled water, and building space is however, greatly reduced. In addition, the annual operating cost of the magnet will be reduced by ~$2M per year.

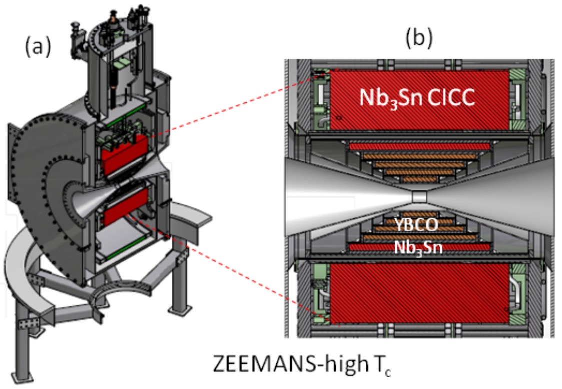

Figure 9. ZEEMANS all superconducting magnet for neutron scattering at the Spallation Neutron Source.

The outsert coil for Zeemans is one of three similar CICC magnets designed by the NHMFL and is similar to magnet designs for ITER. CICC technology was chosen for the outsert coils as they can experience large transients (dB/dt ~ 1 T/s) when the insert magnet trips off. Also the supercritical He in a CICC provides tremendous cooling power against the heating associated with ac losses.

For the inner coil, YBCO coated conductor is nearly the perfect superconductor. It has high critical current up to very high field. Commercial development of YBCO has advanced rapidly motivated by applications at 77 K. YBCO coated conductor is a tape with nominal dimensions of 4 mm width and 0.2 mm thickness for this application. Layer winding is accomplished on a coil form that provides an overall mechanical structure. In 2007 a superconducting coil was tested at the NHMFL. It used an YBCO tape coil provided by SuperPower and set a record field of 7.8 T in a 19 T background for a total of 26.8 T. It was made possible by the new, high-strength, stable YBCO tape Superpower first released in 2006. Additional model coils have been made of superpower tape, demonstrating that it is now possible to design YBCO user magnets.

9. Instrument Performance

The Zeemans instrument as described above provides flux and resolution equivalent to similar SNS instruments. Therefore the capabilities of the existing SNS instrument suite will be provided for use with the high fields. Figure (a-b) show the flux on sample for the diffractometry and spectroscopy configurations, respectively[7]. The values in these plots emphasize the high performance of the instrument.

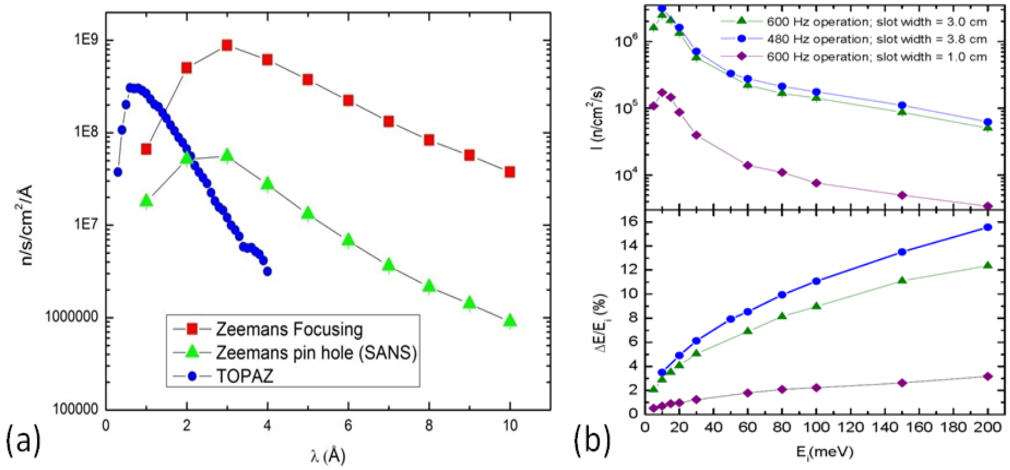

Figure 10. (a) Flux on sample for Zeemans in a full focusing condition and in the SANS pin hole condition. For comparison on the flux on sample for the SNS TOPAZ instrument is plotted. The Flux for both Zeemans configurations is comparable to the respective non-field instrument albeit with ~ 1/3 the bandwidth. (b) Predicted flux on sample and corresponding elastic resolution, for Zeemans operating as a spectrometer. These flux values are comparable to the other direct geometry spectrometers at the SNS.

Zeemans preferentially favors Low Q regions, where magnetic scattering is strong and thus the optimization goal is more long wavelength flux. Figure 10(a) shows that this goal is achieved when compared to TOPAZ[8]. Conversely TOPAZ is superior at shorter wavelength. Likewise, the flux for the pinhole configuration is similar to the flux on the EQ-SANS instrument at SNS.

Figure 10 (b) shows the flux on sample and resolution for Zeemans operating as a spectrometer under several different resolution conditions. The values are comparable to other SNS spectrometers [9-12]. Both a fine resolution mode and two moderate resolution modes are shown. The long initial flight path affords an opportunity to effectively increase the flux further through RRM as discussed earlier. The Zeemans flight path allows for at least 3 sub frames. Thus a multiplication factor of at least 3 can be applied to the flux values in Figure 10 (b).

Another important characteristic of a neutron spectrometer is the accessible momentum transfer (**Q**) range. The **Q** range is controlled by the detector coverage and the degree to which single crystalline samples can be rotated around directions that are perpendicular to the instrumental wave vector transfer[13]. These features are summarized in Figure (a-b) for the white beam diffraction case, where (a) and (b) provide an independent view of the forward and backscattering bank, respectively. Magnetic scattering will be observed in all frames of the forward scattering bank and for frames greater than four in the backward scattering.

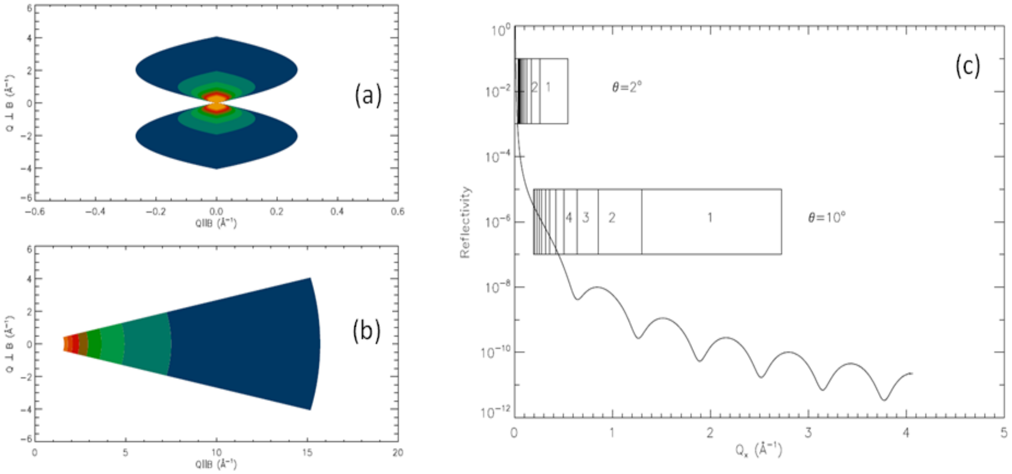

Figure 11. The Q range covered by (a) the forward and (b) the backward detectors of the Zeemans Instrument in diffraction mode. The Q perpendicular to the Field direction is on the vertical axis and the Q parallel to the field direction is on the horizontal axis. The color scale indicates the wavelength frame of operation. (c) A simulated reflectivity curve for 10Å SiO2 on a Si substrate measured on ZEEMANS. The boxes show the Q range covered for a numbered source frame for two different reflection angles.

The **Q** range for the forward scattering bank has its greatest extent along the axis perpendicular to the field. Therefore to appreciably change the **Q** range viewed by the sample, the sample must be rotated primarily about the field axis. These figures show that there is sufficient **Q** range to perform a diffraction experiment. Opening the cone angle would access more of **Q** space but decrease the maximum field significantly. The chosen cone angle is a compromise between field and **Q** range.

Zeemans is also designed for reflectometry. Figure 11 (c) shows a simulated refectivity curve for the standard neutron reflectrometry sample of 10Å SiO$_2$ on a Si substrate. The calculation shows that by tuning the angle of the incident beam with respect to the sample, one can tune the available Q space. For an angle of 10^0 the instrument will be able to reach Q$_x$ > 2.5 Å which means reflectivities well into the background limit of any current state of the art reflectometer. On the other extreme, angles of 2^o or less will allow access to the total external reflection regime.

10. Conclusions

An instrument concept for Zeemans, a high magnetic field beam line at the SNS, has been completed. It incorporates an all superconducting 30T magnet. The instrument is designed to provide excellent performance for Diffraction, Spectroscopy, SANS and reflectometry.

11. Acknowledgements

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