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Design Criteria for the Spallation Neutron Source Instrument Systems Magnetism Reflectometer

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SPALLATION NEUTRON SOURCE
A U.S. Department of Energy Multilaboratory Project
Argonne National Laboratory • Brookhaven National Laboratory • Thomas Jefferson National Accelerator Facility • Lawrence Berkeley National Laboratory • Los Alamos National Laboratory • Oak Ridge National Laboratory
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DESIGN CRITERIA DOCUMENT

MAGNETISM REFLECTOMETER

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DESIGN CRITERIA DOCUMENT

MAGNETISM REFLECTOMETER

CONTENT:

List of acronyms

ANL:	Argonne National Laboratory
CILAS:	Compagnie Industrielle des Lasers (neutron guide manufacturer)
DCD:	Design Criteria Document
IAT:	Instrument Advisory Team
IOC:	Instrument Oversight Committee
IPNS:	Intense Pulsed Neutron Source (ANL)
ISIS:	Pulsed neutron and muon source at Rutherford Appleton Laboratory (England)
HFIR:	High-Flux Isotope Reactor (ORNL)
HMI:	Hahn Meitner Institute
LEED:	Low-Energy Electron Diffraction
MOKE:	Magneto Optical Kerr Effect
NIST:	National Institute of Standards and Technology
NOTS:	Neutron Optics Test Station (ORNL)
ORNL:	Oak Ridge National Laboratory
RHEED:	Reflection High-Energy Electron Diffraction
SNS:	Spallation Neutron Source
SANS:	Small-Angle Scattering
TBD:	To Be Determined
TOF:	Time-Of-Flight
UHV:	Ultra-High Vacuum

0. Introduction

The SNS Instrument Oversight Committee (IOC) recommended in Feb. 2000 the construction of a pair of reflectometers, one specialized in studies on liquid surfaces, the other designed for magnetism studies on thin films. The purpose of this Design Criteria Document (DCD) is to define the requirements for the detailed engineering design of the Magnetism Reflectometer. It is assumed that the reader of this document is familiar with the initial conceptual design study of the SNS reflectometry beamline, which was issued in June 1999 by F. Klose and J. Ankner [1]. Many arguments that have led to certain design choices will not be repeated in this DCD. Although general concepts for both reflectometers have not been changed much since June 1999, there are specific areas where changes have been made. Wherever the design is modified compared to the conceptual design study, the reason is explained.

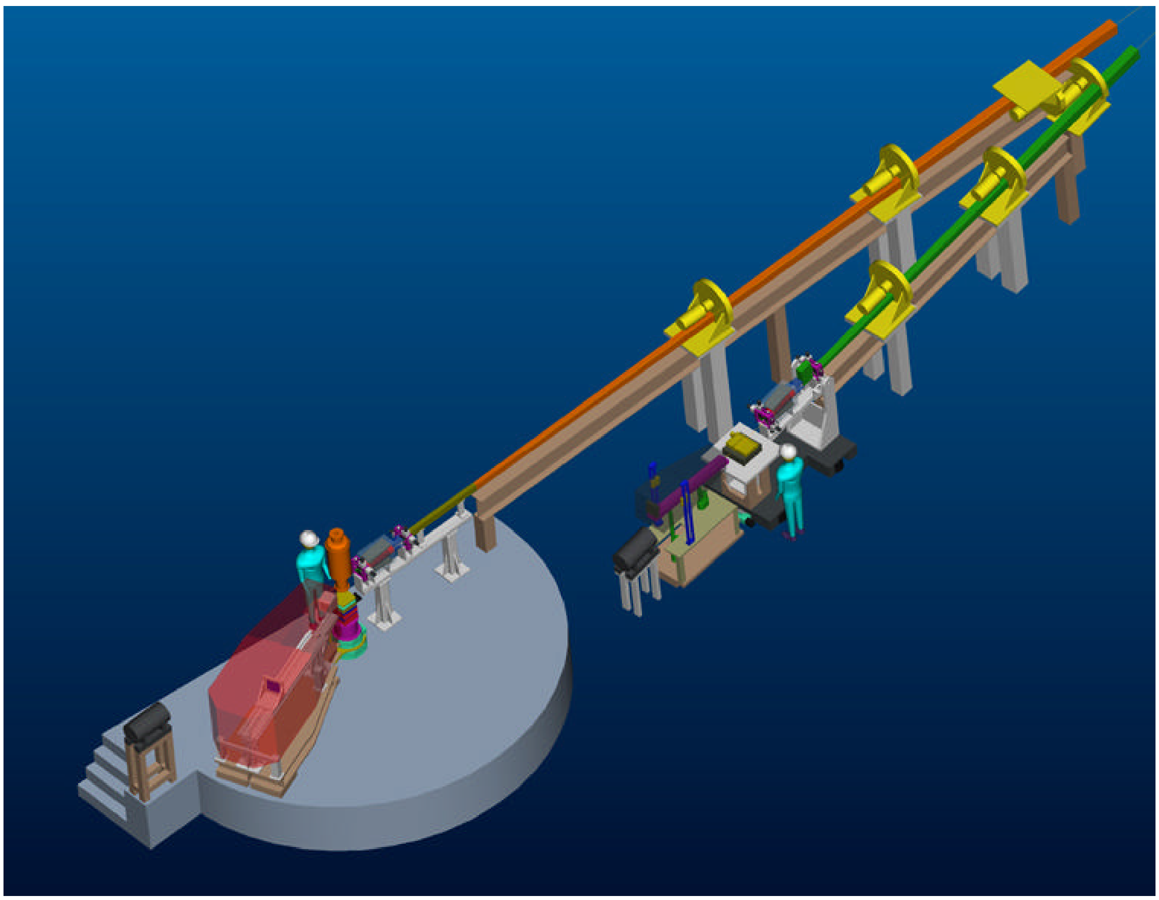

Fig. 1: The SNS reflectometry beamlines: The upper beamline represents the Magnetism Reflectometer, the lower the Liquids Reflectometer.

The main outcome of our conceptual design study was a demonstration of the feasibility of locating two reflectometers on a single beam port, without compromising the performance of either instrument. The instruments look at the same moderator through a single primary beamline shutter. In order to achieve optimal instrument performance, it was necessary to alter the initial shutter design, such that two individual optics for beam extraction would fit. The most important conclusion of our study was that the dual instrument concept required only minor compromises in the individual instrument designs, i.e. the instruments would look almost the same if one would attempt to build them on separate beam lines. However, during all decisions concerning the detailed engineering design of the Magnetism Reflectometer, it should be kept in mind that the Liquids Reflectometer will be build in close proximity (see Fig. 1). The main area where compromises are necessary concerns sharing the available space within the beam line.

The Magnetism Reflectometer, presented in this document, is a neutron scattering instrument designed mainly for reflectometry and high-angle diffraction studies on magnetic thin films and surfaces. The availability of polarized neutrons and the polarization analysis capability suggests that the instrument will also be used for specific studies on non-magnetic thin film samples. Examples for the latter cases include contrast variation, incoherent background reduction and phase determination for direct inversion of reflectivity data into real-space scattering-length density profiles.

The basic layout of the instrument is illustrated in Figure 2. Neutrons from the moderator are guided to the sample position at a 17.5 m distance via a combination of a short channel beam bender and a tapered neutron guide. Neutrons that are reflected/diffracted by the sample will be counted by a two-dimensional multidetector at a 19 m distance from the moderator. Polarizing neutron optical elements (polarizer, analyzer and spin flipper) determine the spin-state before and after scattering on the sample. The wavelength is determined by time-of-flight. The instrument is designed for 60 Hz operation. Bandwidth choppers restrict the total bandwidth of neutrons that are incident onto the sample to $\Delta\lambda$ = 3.5 Å when the instrument is collecting data in every time frame. Since the moderator intensity peaks at a wavelength of 2.5 Å and the guide transmission increases linearly with wavelength from approximately 2 Å (see section 2), the highest intensity will be available in the second frame (3.5 Å - 7.0 Å). However, by changing the phasing of the bandwidth choppers, the available 3.5 Å bandwidth can be shifted to either smaller or higher neutron wavelength. Additionally, by changing the speed of the choppers, pseudo 30 Hz (or lower) operation can be realized with correspondingly wider wavelength bandwidth.

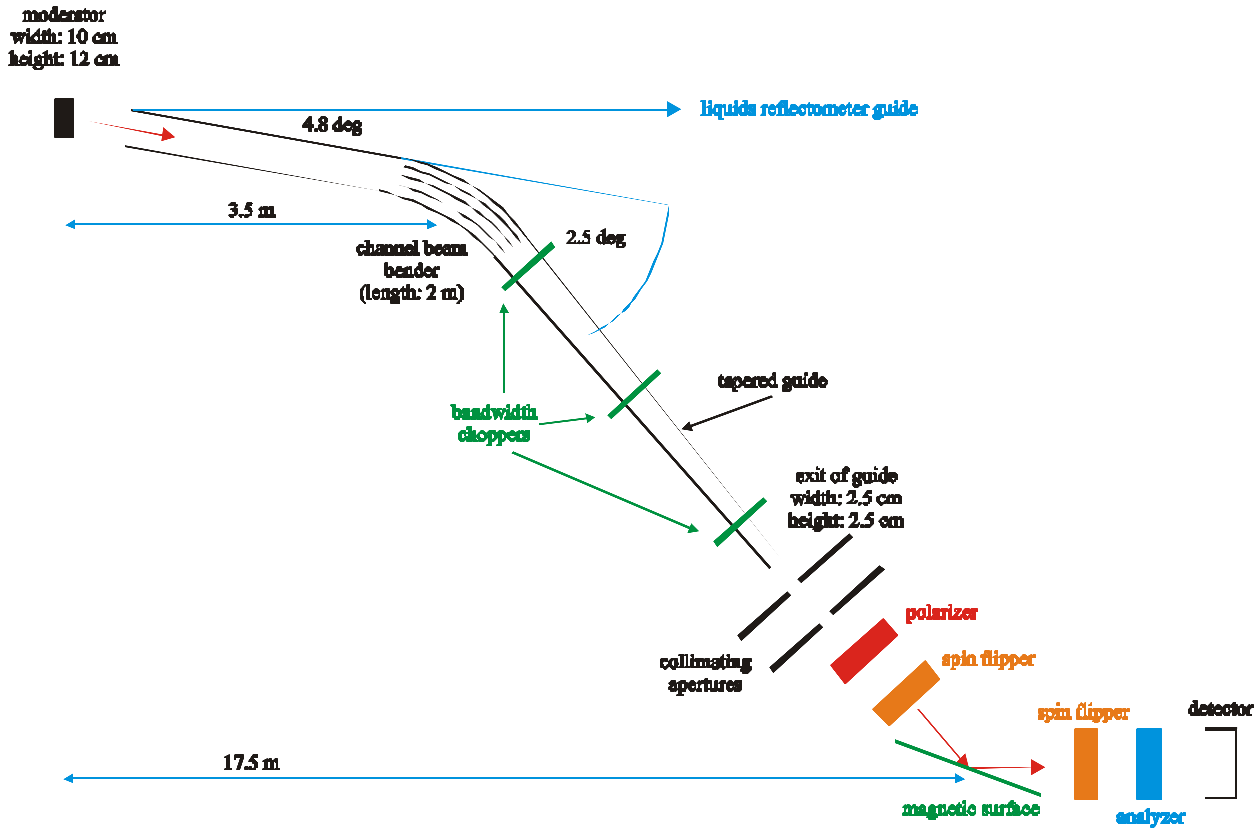

Fig. 2: Neutron beam optics of the magnetism reflectometer (top view, schematic).
The microchannel deflector (beam bender) bends the beam out of the direct-line-of-sight to the moderator.

Due to the small amount of material that interacts with the beam, scattering experiments on thin films (reflectometry and high-angle diffraction) are generally countrate/background limited. For certain reflectometry experiments, it is desirable to measure signals in the 10^{-10} range relative to the neutron flux incident on the sample surface. Thus, shielding and background reduction have very high priority for this instrument. In order to address these critical issues, a short beam bender (followed by a tapered neutron guide) has been chosen as an integral part of the neutron transport system.

The instrument is primarily intended to be used for *elastic* scattering experiments. It needs to be examined if the expected signal-to-noise ratios will allow *inelastic* measurements on thin film structures.

The design criteria for the instrument will be described in the following main sections:
1. Operating Modes, 2. Neutron Transport System, 3. Chopper System, 4. Detector and Data Acquisition System, 5. Polarization Handling, 6. Sample Environment, and 7. Shielding.

1. Operating Modes

1.1 Polarized reflectometry

Polarized reflectometry is the main operating mode of this instrument. The goal in polarized reflectometry experiments is to determine magnetic and structural depth profile of thin films and multilayers [2].

One of the first choices that needed to be made was to decide on the basic scattering geometry, i.e. either to choose a horizontal or a vertical sample geometry. The horizontal sample geometry is less suitable since it is not compatible with conventional cryostat and magnetic field configurations. Superconducting magnets that will be used as one of the standard sample environments usually have a vertical field axis. Furthermore, it would be, from an engineering standpoint, very difficult to provide for a vertical movement of the secondary instrument axis (analyzer optics bench, detector and shielding), especially for the planned high-angle diffraction experiments. For the latter case the angle between incoming beam and detector axis can be as large as 160 deg.

Due to these considerations, a horizontal scattering geometry (with a vertical sample surface) has been chosen. In this geometry the detector assembly can be moved very easily on a horizontal floor, by means of air cushions or a rail system, for example. The drawback of this arrangement is that the two instruments do not fit exactly next to each other (Also from a practical point of view one would not like to have the sample positions exactly next to each other. Independent operation of the two instruments, for example the loading of samples, would not be possible in such a configuration.). Thus, we have decided to move the Magnetism Reflectometer further outward. The sample position will be located at 17.5 m distance from the moderator, even though the available wavelength bandwidth is reduced. The general layout of the instrument is shown in Fig. 3.

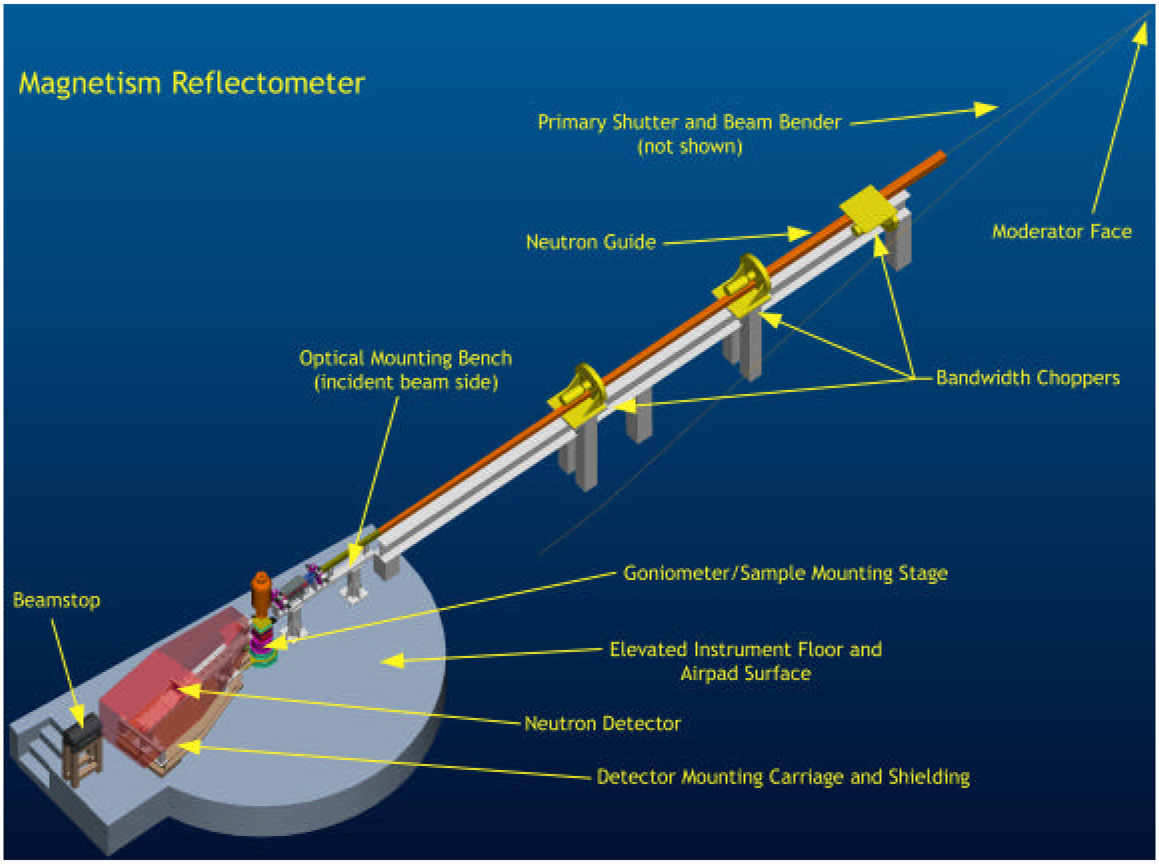

Fig. 3: The Magnetism Reflectometer consists of the following components: channel beam bender (not shown), tapered neutron guide, bandwidth choppers (yellow), polarizing optics, sample area (with a cryostat mounted), detector assembly (analyzing optics, detector, shielding) and a beam stop.

Another important point that strongly favors a longer instrument is the requirement to guide smaller neutron wavelengths to the sample for the planned high-angle diffraction experiments. A useful bender cut-off wavelength would be 1.8 Å. This number implies that one cannot deflect the neutron beam with a 2 m channel bender by 2.0 deg as it is planned for the Liquids Reflectometer (see section 2.3 for further discussion). Thus, a larger direct-line-of-sight length and a correspondingly longer minimum instrument length is required for the Magnetism Reflectometer.

Since the design is optimized based on intensity considerations for 60 Hz operation, only a relatively small wavelength band ($\Delta\lambda$ = 3.5 Å) will be used. Data can be collected in three wavelength frames (0 Å - 3.5 Å, 3.5 Å - 7.0 Å, or 7.0 Å - 10.5 Å) by proper phasing of the neutron choppers. If it turns out that the prompt pulse does not introduce too much background, one can also shift the wavelength band $\Delta\lambda$ = 3.5 Å across the frame borders, e.g. one could use the high-intensity region from 1.8 Å - 5.3 Å. The variable of interest is the scattering vector **Q** ($Q = 4\pi \sin\theta / \lambda$, with θ: scattering angle). The desired Q-range needs to be scanned by several angular settings. For a complete specular reflectometry experiment one will need about 10 different settings [3]. In this respect, the instrument can be regarded as a hybrid between typical broad wavelength band TOF instruments like POSY at IPNS or CRISP at ISIS, and monochromator instruments like NG-1 at NIST or ADAM at ILL. While the former instrument types require typically 3 or 4 angular settings, the latter need up to several hundred settings for a complete reflectivity scan.

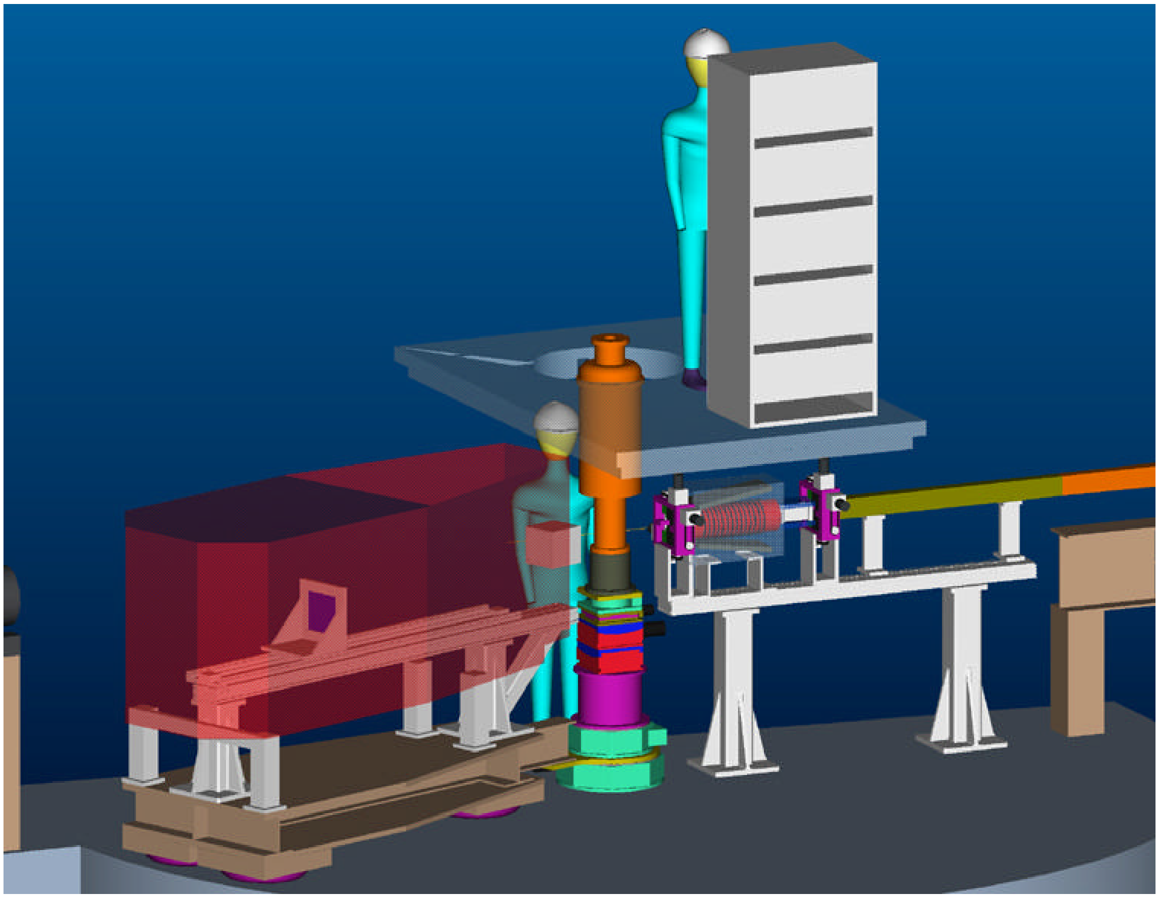

Fig. 4: Detailed view of the beamline close to the sample position. If a cryostat is in use, sample loading will be done from a platform atop the sample area. Otherwise sample access is possible from the instrument floor

In the reflectometry mode, the angular collimation within the scattering plane will be defined by two aperture systems, approximately 1 m apart from each other (although for high scattering angles a stacked collimator system might provide a better illumination of the sample, see below for details). The neutron guide system will be designed such that even for the smallest available neutron wavelength (approx. 1.8 Å) a high angular divergence (approx. +/-1 deg.) will be transported onto the sample (see also section 2). A transmission polarizer system and a spin flipper (see below) will be placed between the apertures. All elements will be mounted on an optical bench. On the secondary side of the instrument there will be a neutron spin flipper, an analyzer, the detector and finally a beam stop (for details see section 5). In order to design the optical elements, a typical sample size has to be determined. A sample area of 25 mm x 25 mm has been chosen as a useful compromise. This size determines the exit size of the tapered neutron guide. Fig. 4 shows a detailed view of the instrument components close to the sample position.

1.2 Polarized high-angle diffraction (scattering vector perpendicular to sample plane)

This operation mode is used to determine the magnetic and chemical structure perpendicular to the sample surface on atomic length-scales. In order to achieve high intensities in high-angle diffraction experiments one needs to take into account that the required horizontal beam size is not extremely small, as is the case for reflectometry experiments, but approaches the full length of the sample. This fact sets the horizontal exit size of the tapered guide to 25 mm.

For the high-angle diffraction mode of this instrument one needs to consider that thin films and multilayers often show, compared to bulk samples, much broader diffraction peaks. While the weakest collimation that is generally used in high-angle diffraction experiments on bulk samples is on the order of 1% - 2%, this instrument might benefit from an even weaker collimation in order to make up for the low intensities inherent to thin film samples.

At high scattering angles the incident beam divergence will not be defined by slit apertures, but by stacked collimator systems (before and after the sample) that offer much higher intensity. A new concept for wavelength dependent collimator systems has recently been developed by Th. Krist et al. [4]. This collimator type offers higher transmission compared to standard collimator systems and is our preferred choice.

Fig. 5 shows a typical instrument setting for high-angle diffraction experiments.

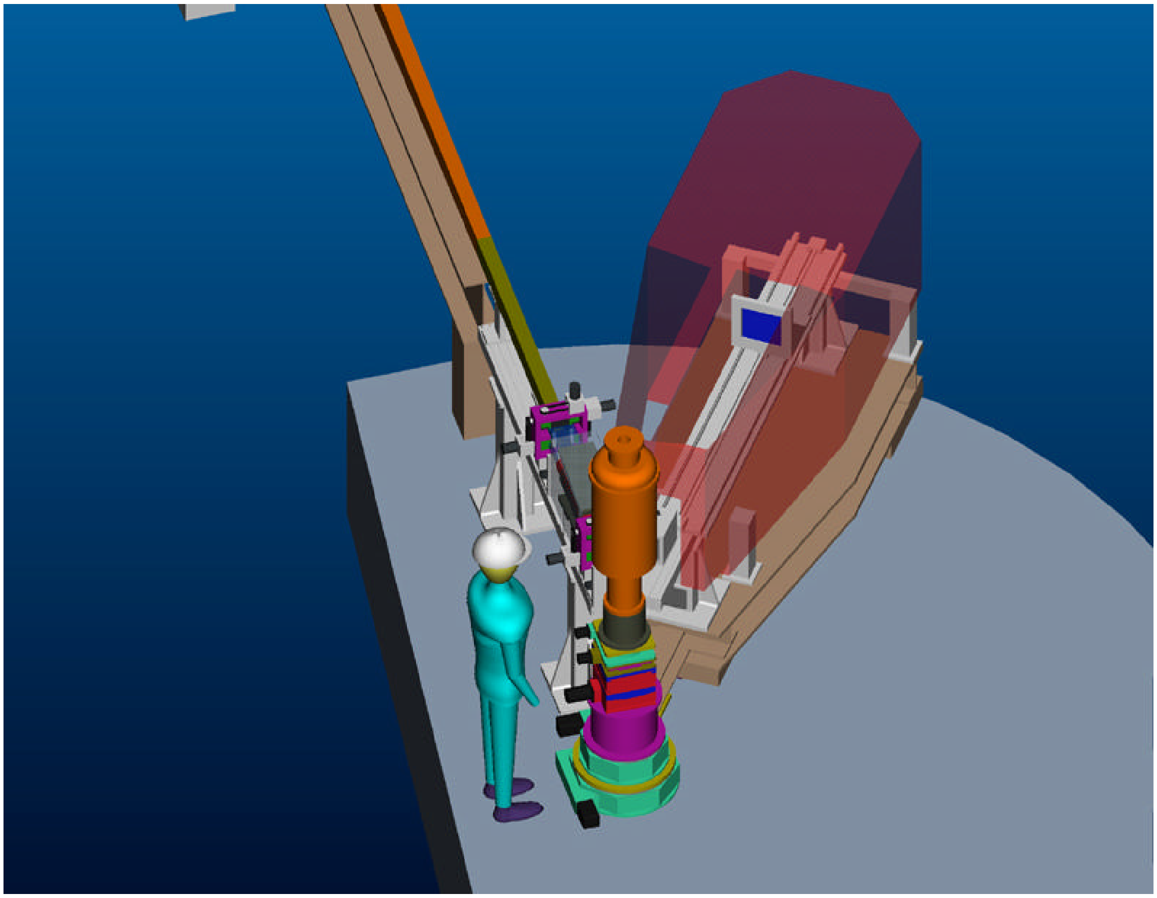

Fig. 5: Instrument in high-angle diffraction mode.

1.3 Polarized grazing-incidence diffraction (scattering vector within the plane of the sample)

This operation mode will be used to determine atomic or large-scale magnetic/chemical periodicities within the sample plane. There are two possibilities for the overall sample/scattering geometry:

(i) One could use a vertical sample surface geometry and move the detector in a vertical plane.

(ii) One could use a horizontal sample surface geometry and move the detector in a horizontal plane.

It should be noted that in commercial X-ray diffraction systems with grazing incidence in-plane diffraction capabilities, both possible experimental arrangements are realized. RIGAKU prefers to keep the sample in the same vertical position as in reflectometry experiments, while the PHILIPS and BRUKER systems turn the sample surface from the vertical into a horizontal position by means of a Eulerian cradle (see appendix). For the SNS Magnetism Reflectometer, an Eulerian cradle solution would be very attractive, even though there is some doubt if a magnetic field configuration of sufficient strength can be achieved in this design.

The simplest method to change from a vertical sample surface geometry (used for standard reflectometry experiments) to a horizontal sample surface arrangement is to manually change the sample orientation. For this purpose, the cryostat should have two different sample mounts, one for vertical and another for horizontal sample orientation. Required changes of magnetic field directions can be achieved either by motorized movements of the sample magnet or by using a special magnet with three field axes (see section 6.3).

2. Neutron Transport System

The neutron guide system will consist of a channel beam bender and a tapered neutron guide. The bender is used to get out of the direct-line-of-sight to the moderator over a relatively short distance, while the tapered guide is used to focus as much neutron flux as possible onto the sample. For an optimal design of these guide components, the performance of the moderator has to be considered. Details of the guide dimensions and geometry are provided in Table 1.

Internal Dimensions	Guide Type	Coating	Starting Position	End Position	Internal
10 cm (H) x 12 cm (V)	flight tube, absorbing walls	no coating	1.00 m	2.50 m	^{4}He
10 cm (H) x 12 cm (V)	horiz.beam bender 6 channels	3.6 x θ_c Ni (H) 3.6 x θ_c Ni (V)	2.50 m	4.50 m	^{4}He
10 cm (H) to 3 cm (H) x 12 cm (V) to 3 cm (V)	tapered neutron guide	3.6 x θ_c Ni (H) 3.6 x θ_c Ni (V)	4.50 m	16.50 m	Vacuum

Tab. 1: Characteristics of the guide system: Starting and end positions are given relative to the moderator face and along the nominal center of the neutron beam path as defined by the internal surfaces of the guide.

Because of the high neutron flux internal to the target monolith, all mirror support material for guides located within the direct-line-of-sight length must be of either metal or a non-boron containing glass. External to the target monolith a boron containing glass is the preferred substrate material due to its neutron absorbing characteristics.

The combination of the SNS high-intensity cold moderator and this high-performance neutron guide system will result in a time-averaged cold neutron flux that is comparable to corresponding values of the best reactor facilities like ILL or NIST. Fig. 6 shows the calculated neutron flux of the SNS Magnetism Reflectometer at the exit of the neutron guide system at 1 m distance to the sample (Monte Carlo calculation based on the parameters given in Tab. 1. In this calculation a reflectivity of 70 % has been assumed at 3.6 x θ_c Ni).

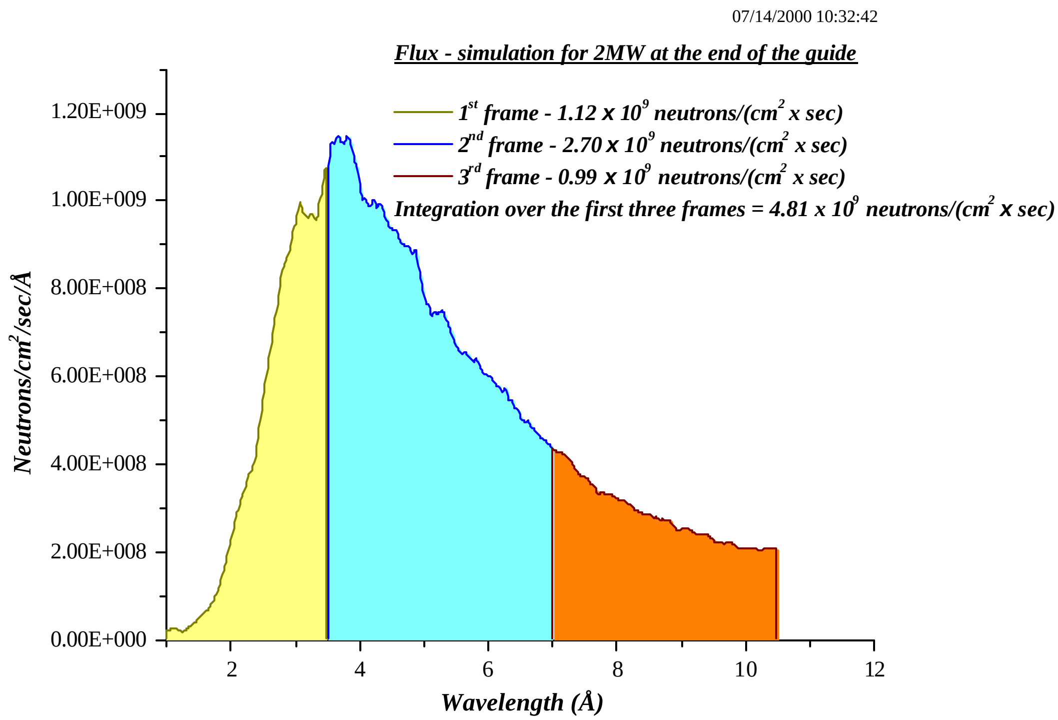

Fig. 6: Calculated neutron flux at the exit of the tapered neutron guide of the SNS Magnetism Reflectometer. Note that the flux is pulsed with a frequency of 60 Hz and has an intrinsic time/wavelength resolution of 0.4% (see also section 2.1).

The reflectometer with the highest continuous neutron flux on sample is the redesigned D17 at ILL (integrated cold neutron flux of 9.6 x 10^9 neutrons/cm^2/s) [5]. In contrast, the neutron flux of the SNS Magnetism Reflectometer is pulsed. At 19 m instrument length, a bandwidth of 3.5 Å can be used. If, for example, the second frame is used for data collection (see Fig. 6), a neutron flux of approximately 2.5 x 10^9 neutrons/cm^2/s can be achieved on the sample with an intrinsic time/wavelength resolution of 0.4 %. Therefore, typical gain factors compared to current state-of-the-art reflectometers like D17 will be in the range of one to two orders of magnitude. The exact gain will depend on the resolution and other experimental requirements (see also Ref. [3]).

2.1 Moderator

The Q-resolution requirements for the Magnetism Reflectometer are strongly sample dependent. The extremes range from less than 1% for films several thousend Å thick to 10% or even 15% if monolayer films are studied (for the majority of experiments, one expects medium resolution requirements). Depending on the required resolution and Q-range, the operating neutron wavelengths of this instrument are 1.8 Å $< \lambda <$ 10.5 Å , with primary emphasis in the λ = 3 - 4 Å region. The lower bound is dictated by the cut-off wavelength of the bender, the upper bound mainly by the chopper system characteristics and intensity considerations.

The moderator that best suits our needs is the top downstream cryogenic moderator (supercritical H_2 at ≈22 K). For this coupled moderator the emission-time uncertainty increases monotonically over the reflectometer's usable wavelength range (see Fig. 7). For the overwhelming majority of experiments, one does not require a timing resolution better than $dt/t = dl/l = 0.01$. Simulations of the expected performance of the coupled H_2 SNS moderator by Erik Iverson indicate that its timing resolution is more than a factor of two smaller than needed for the 19 m long instrument. The users of this instrument would therefore welcome a broader emission-time spectrum, particularly if accompanied by a greater-than-linear increase in flux.

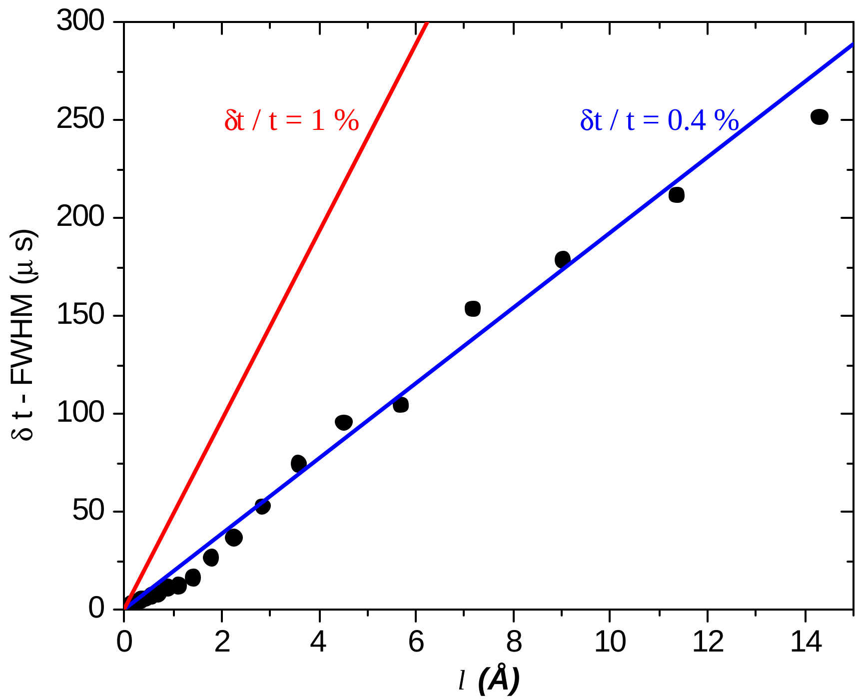

Fig. 7: Simulated moderator emission-time (solid circles, FWHM values, from E.B. Iverson) as a function of wavelength. The 19 m long Magnetism Reflectometer could tolerate a broader $dt/t = 0.01$.

It is clear that changes in the moderator pulse width will modify the instrument performance (intensity can only be gained at the expense of the time resolution). Since the Magnetism Reflectometer includes a neutron-spin polarizer/analyzer system and a Drabkin spin-resonance energy filter (see section 5.6), it would even be possible to recover from the resolution loss that would result from using a moderator with longer emission time.

After various discussions with SNS Target Systems, it was decided to locate the necessary extra wide main experiment shutter on beam line 4. The Magnetism Reflectometer will occupy sector 4A of the beam line. Note that the location of the reflectometry beamlines has been changed from the assignment reported in the CDR since the overall moderator arrangement was changed for optimization reasons. Fig. 8 shows a plan view of the target monolith / wide shutter area.

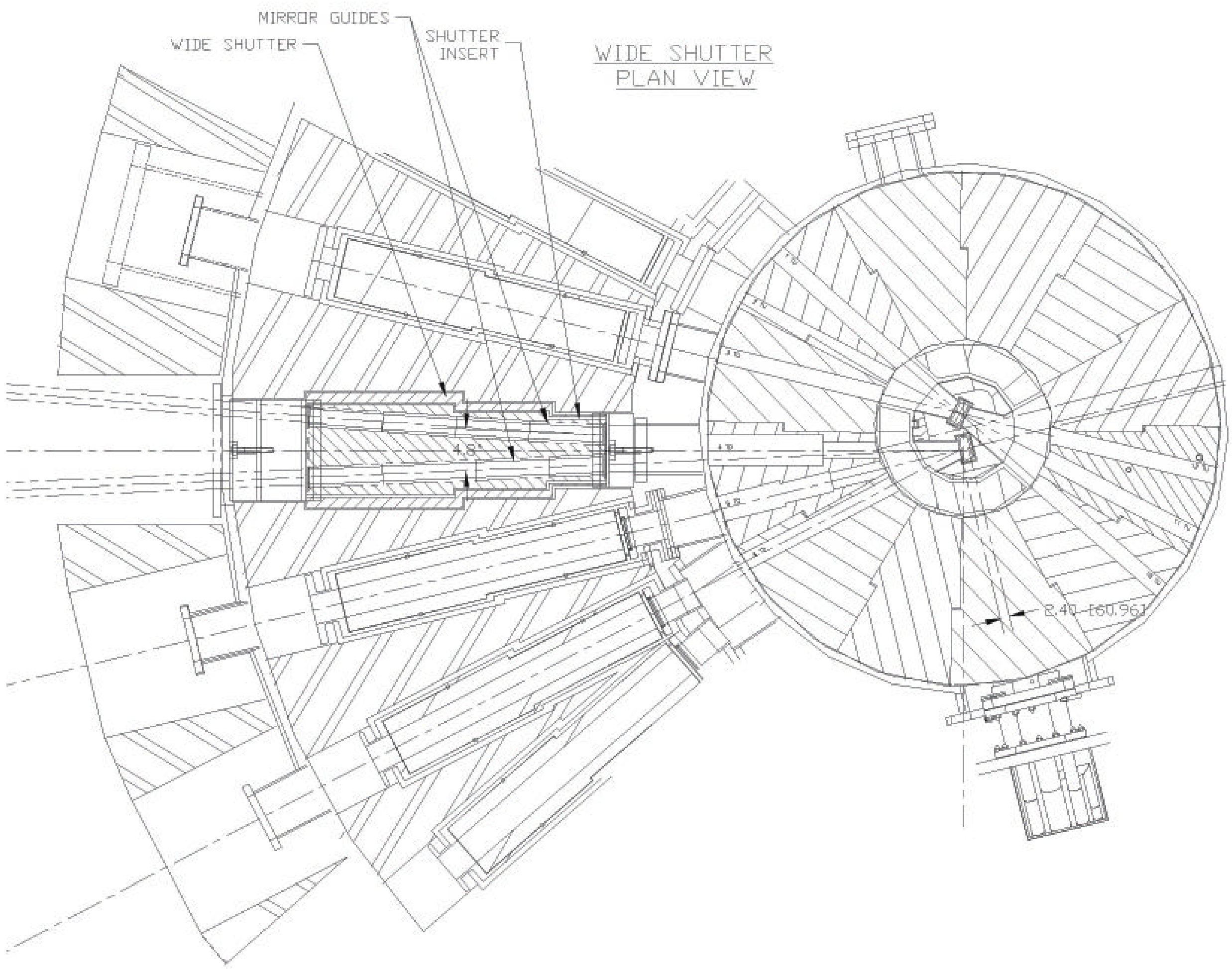

Fig. 8: Moderator / wide shutter configuration on the SNS reflectometry beamline.

2.2 Moderator / neutron guide coupling

Preliminary Monte Carlo simulations of the neutron beam transport system suggest that there is little gain in using neutron guides very close to the moderator, specifically in the core vessel insert region which is located between the shutter and the moderator (1 m to 2.5 m from the moderator face, see Fig. 8). Furthermore, one would expect severe radiation damage of components in this region close to the moderator due to the corresponding high flux of high-energy neutrons and γ-rays. In our current design the 10 cm (width) x 12 cm (height) moderator is connected by only a flight tube with absorbing/shielding walls (material: TBD) to the entrance of the beam bender at 2.5 m distance. This section internal to the core vessel region will be filled with ^{4}He. The capability for continuous flow at TBD cfm of ^{4}He gas at ambient temperature is required.

2.3 Channel beam bender

The short channel beam bender is one of the key elements in the design of the neutron transport system. Its main purpose is to steer the neutron beam out of the direct-line-of-sight to the moderator (the main source of background radiation) relatively quickly in order to maximize space for shielding material between the area where the unwanted high-energy radiation hits parts of the beam line and the sample/detector area. Such short beam benders became available only recently due to improvements in supermirror guide coatings. Several actual systems built at different facilities (e.g. at Paul Scherrer Institute and at NIST) are working close to their theoretical predictions. No particular problems have been reported concerning secondary emission of background while such systems are used within the direct-line-of-sight to a moderator. Ni/Ti supermirrors with m = 3.5 (produced at PSI) have been tested recently for radiation stability [6]. No change in reflecting properties have been reported for an integrated thermal neutron flux of 10^{19} neutrons/cm^2 (at the location of the irradiation channel close to the core of a nuclear reactor, a flux of 3 x 10^{13} thermal neutrons/cm^2/sec and 8 x 10^{11} fast neutrons/cm^2/sec was present). Additional irradiation tests on neutron optical elements are currently under way at IPNS.

Fig. 9 shows the channel beam benders of both instruments integrated into the main beam line shutter. The bender for the Magnetism Reflectometer is the upper one, which bends the beam horizontally. In the current design, the bender curvature is achieved by four straight sections, each with an offset of 0.5 deg. It should be noted that, in general, the main beam line shutter will not be used for blocking the neutron flux to the sample. This operation will be provided by an auxiliary instrument shutter (see section 7.3). The main shutter will only be used if instrument components within the direct-line-of-sight need to be accessed (example: exchange of a chopper system while SNS is running).

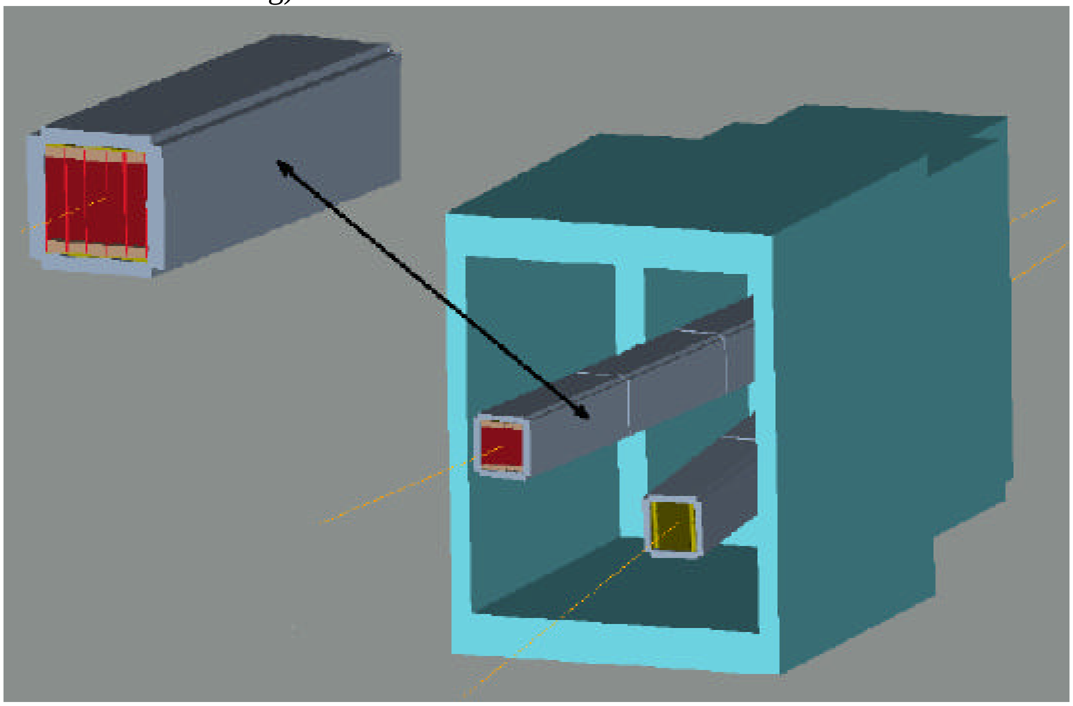

Fig. 9: Schematic representation of the channel beam benders integrated into the main beamline shutter. One of the four straight bender sections is depicted enlarged.

An alternative design for the general neutron transport system could consist of a so-called "T_0 chopper" and a following curved guide. A T_0 chopper consists of a rod of neutron absorbing/scattering metal alloy (often Inconel is used) mounted on a rotating disk that is driven into the beam at the time when the proton pulse hits the target. Since the T_0 chopper assembly needs to be rotated with the same frequency as the source (60 Hz), the weight of the rod needs to be restricted. In practical designs, the rod has a typical length of only 30 cm. In contrast, our neutron guide design has a minimum shielding length of more than 2 m in the area that is out of direct-line-of-sight, i.e. a much better shielding performance can be expected. Additionally, because of space limitations due to extracting two beamlines from a single beamport, fitting two T_0 choppers near the target monolith is nearly impossible.

Preliminary Monte Carlo simulations have been carried out for the Magnetism Reflectometer with an assumed total instrument length of 19 m. According to these results, we propose the following bender design:
(The final specifications for bender geometry and materials will be made based on the recommendations of experts who have actually manufactured and tested real devices.)

- Overall length: 2-4 m
A short bender would help to get out of direct-line-of-sight earlier. For a 2 m long bender with 2 deg. deflection and a following tapered guide system that provides another 0.5 deg. beam deflection, one can lose direct-line-of-sight after 8.5 m [1]. A longer bender, however, has a smaller cut-off wavelength. Due to the planned high-angle diffraction experiments, a cut-off of less than 2 Å would be desirable. This can be better achieved with a longer device, e.g. of 4 m length. The drawback would be that the bender needs to be split into two parts, since there is not enough space for mounting the complete device inside the 2 m long shutter. Further optimization of the bender could also be achieved by making the extracted beam width smaller. Certainly, this would reduce the intensity on the sample, but it would possibly also increase the signal-to-noise ratio, since for many experiments an extremely high beam divergence (which is created by the tapered guide following the bender) is not needed.

- Number of channels: approx. 6
Simulations show that the transported neutron flux at the sample cannot be significantly increased by further increasing the number of beam channels beyond a certain value (for a given bender geometry). 4 - 6 channels are typical numbers for achieving an optimal performance/cost relation. The channel thickness that was assumed in the Monte Carlo simulations was 0.5 mm. This value is typically used in the construction of actual beam bender devices. The most cost-effective material is non-boron containing float glass.

- Vertical guide coatings: $m \geq 3.6$, reflectivity ≥ 70% at the critical edge
A guide coating with $m = 3.6$ with a reflectivity of 70 % at the critical edge is the best commercially available today ($m = 4$ supermirrors are available only as prototypes). The better the coating, the smaller the cut-off wavelength for a given bender geometry, which will increase the performance in high-angle diffraction experiments.

- Horizontal guide coatings: $m \geq 3.6$, reflectivity ≥ 70% at the critical edge

Since the sample surface of the Magnetism Reflectometer is vertical, reflectometry experiments can be carried out with a very high vertical divergence. Thus, the horizontal guide coatings should be as highly reflecting as possible for achieving high intensities.

Fig. 10 shows the wavelength-dependence of the beam divergence at the exit of the tapered neutron guide (calculation based on parameters from Tab. 1).

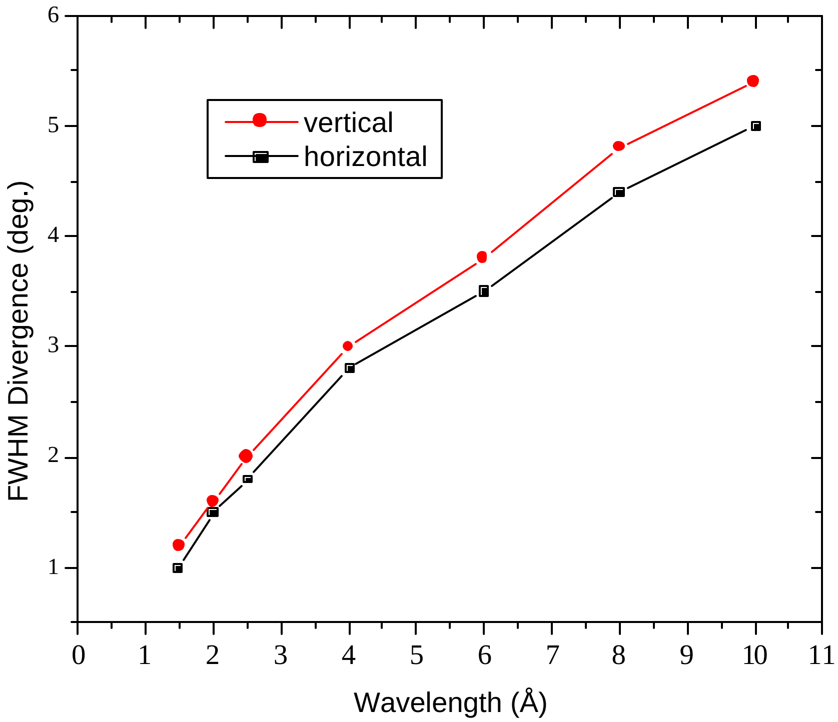

Fig. 10: Wavelength-dependence of the beam divergence at the exit of the tapered guide.

- Testing

Since the bender optic is the key optical element of the neutron transport system, one needs to be sure that it is working close to its theoretical limit. Thus, neutron beam testing must be carried out before installation of the device into the SNS Magnetism Reflectometer beam line. It is foreseen that these tests will be carried out at the SNS neutron optics test station (NOTS) at ORNL's HFIR reactor.

- Installation, alignment & operation

Both channel benders will be incorporated into a common shielding assembly. This assembly will float within the main beam line shutter (see Fig. 9). Precision supports will provide a highly reproducible alignment of the benders relative to the other parts of the neutron guide. The required reproducibility of the bender alignment is in the order of a few 1/100 deg. During operation the channel bender system will be filled with ^{4}He. For cooling purposes the capability for continuous flow of ^{4}He gas at ambient temperature may be required.

It should be noted that the "floating beam bender" concept will be evaluated far in advance of actual installation of the device into the Magnetism Reflectometer beam line. The corresponding tests will be carried out at the planned SNS design verification test stand.

2.4 Tapered neutron guide

The main purpose of the tapered neutron guide is to transport as much useful neutron flux to the sample position as possible. Since it is planned to perform diffraction measurements with the scattering vector pointing in different directions both horizontal and vertical guide coatings must have the capability to transport a highly divergent neutron beam to the sample. For example, in the case of out-of-plane reflectometry or diffraction measurements (with vertical sample surface), one can tolerate a very high vertical divergence that will lead to a strong increase in intensity. In addition, for some reflectometry experiments, the horizontal angular resolution can be relaxed to 10% - 15%, even for the shortest neutron wavelength used (1.8 Å). This operating mode also requires highly sophisticated vertical guide coatings (side walls of the guide).

The data for the guide coatings given below represent the state-of-the-art in current commercially available materials. The arguments given above indicate that, at least for the horizontal (top and bottom of the guide) one would benefit from even more advanced coatings. Preliminary Monte Carlo simulations indicate that there is indeed a clear gain in using such high m-value coatings. However, some further optimization needs to be done before a final decision can be made.

- Vertical guide coatings: m ≥ 3.6, reflectivity ≥ 70 % at the critical edge

- Horizontal guide coatings: m ≥ 3.6, reflectivity ≥ 70 % at the critical edge

- Testing

The quality of the guide sections (reflectivity, flatness and geometry) needs to be examined before the individual guide sections can be mounted together to form the tapered guide. It is foreseen that these tests will be carried out at the SNS neutron optics test station (NOTS) at ORNL's HFIR reactor. Additional non-neutron testing will be carried out at the SNS optics lab (X-ray reflectivity/diffraction, LASER interferometry, atomic force microscopy). Certainly, the guide manufacturer will be held responsible for quality assurance of guide section manufacturing.

- Installation, initial alignment and re-alignment after floor settlement

The 12 m long tapered guide will be pre-mounted in two 6 m long sections. The support structure of each of these sections will be very robust mechanically. The individual guide sections will be aligned with high precision on the steel frame (The exact precision requirements will be determined from the general guidance that not more than 5% flux should be lost by random misalignments of the sections. Typical specs used by CILAS usually guarantee alignment to be within a tolerance of 1/100 deg.). It can be assumed that the alignment of the guide sections relative to the steel frame will not change significantly while the instrument is in use. Thus, no extraordinary provisions (i.e. a motorized alignment system) are necessary that will allow realignment of the individual 1 m long guide sections.

The two 6 m long tapered guide sections will be aligned relative to the channel bender. Each of the steel girders that carry the guide assemblies will rest on two support posts located near their ends. The posts should provide a mechanism that allows for precision height and lateral adjustment (see Fig. 3).

Long-term guide alignment is a crucial issue, particularly with regard to differential settlement between parts of the beam line. For example, an abrupt offset of 5% of the vertical guide dimension will diminish the neutron flux on sample by approximately 5%. Random variations in the guide vertical alignment due to changes in floor loading (e.g. as additional instruments are installed) will also cause neutron beam loss if the guides are supported from the floor. Although it is currently planned to prevent significant floor settlement by supporting the experiment hall floor with a system of micro piles, the system design must provide for an easy realignment of the neutron guide system.

A reasonable estimate of the allowed random variation, $\Delta\theta_{vert}$, in the vertical direction before realignment becomes necessary is ~5% of the critical angle for the shortest wavelength neutron (1.8 Å) expected to propagate in the guide:

$$\Delta\theta_{vert} = 0.05 \text{ x } 1.8 \text{ Å x m x } 0.1 \text{ deg./Å} = 0.032 \text{ deg. (for m = 3.6 coating)}$$

Given guide support posts located at 6 m intervals, this translates into a maximum variation in vertical position of the posts of ± 3.4 mm. This number is relative to the vertical position of initial alignment. Manual realignment of the guide system is expected to be time intensive since it involves removal of beamline shielding. It is unreasonable to request manual realignment on a more frequent time interval than 1 year. If deviations on the order of those specified above are expected to occur on a shorter time scale than 1 year then remote vertical realignment capabilities must be engineered into the guide system supports.

Three bandwidth chopper systems will be placed at different positions along the tapered neutron guide. The required notches in the guide will be about 2 cm wide. It needs to be determined if the vacuum containment of the bandwidth choppers will be integrated into the guide vacuum or if the guide sections will be sealed with thin windows (i.e. Al foil).

2.5 Maintenance of the neutron guide system

2.5.1 Vacuum system

In order to maintain as clean as possible vacuum conditions in the neutron transport system, dry pump systems are to be used wherever feasible. This is particularly important for the tapered guide system and for the chopper vacuum lines. During operation of the beam line, the vacuum in the guide should be better than TBD Torr.

2.5.2 Exchange of components integrated into the guide system

In order to limit the amount of windows along the neutron flight path, it is planned to incorporate the choppers in the same vacuum enclosure as the guides. Any removal of the chopper systems, for example for maintenance, must not cause misalignment of the guides. Therefore the choppers must rest on their own support structure, and bellows that are used to connect the chopper vacuum to the guide vacuum must be flexible to prevent any deflection of guide parts. The same precautions should be taken for any other device that is in physical contact with the guide system.

2.6 Aperture systems

Two aperture systems will be used to define the divergence of the neutron beam. Both systems must allow a precise beam collimation in the horizontal as well as in the vertical directions. The former mode is required for standard reflectometry experiments while the latter will be used in grazing incidence diffraction experiments. The movements of the slit blades must be motorized and highly reproducible (1/100 mm). The maximum opening in the vertical and horizontal directions must clearly exceed the exit size of the tapered guide (25 mm x 25 mm). Materials and thickness: TBD.

Sufficient distance must be maintained between the auxiliary beam shutter at the end of the tapered guide and the first aperture system. This space will be necessary for setting up a mirror that will reflect an alignment laser beam into the nominal neutron beam axis.

2.7 Collimators

Collimator systems will be used on the incident as well as on the secondary side of the instrument for the high-angle diffraction modes (in-plane and out-of-plane diffraction). The basic needs are discussed in the sections 1.2 - 1.4. Current plans include the use of 3 different collimator assemblies in order to match different resolution requirements. Note that the collimator system must be rotated by 90 deg. when changing from an out-of-plane to a grazing incidence in-plane diffraction setup. This movement needs to be precise and motorized. Required angular acceptance and materials will be determined by means of Monte Carlo simulations.

There are new developments at NIST and at HMI Berlin in the field of collimators. In order to achieve higher transmission values "stacked" collimator systems fabricated from thin Si plates might be used beneficially [4]. By using a special coating sequence of reflecting and absorbing materials, the divergence angle can be made proportional to the wavelength, which would be very desirable for TOF experiments. These developments need to be evaluated before a final design decision can be made.

3. Chopper System

3.1 T_0 chopper

Neutron scattering instruments, which have a direct view onto a moderator face, usually contain a T_0 chopper in an early upstream position for background suppression. Since the design of the Magnetism Reflectometer's neutron guide system includes a channel beam bender to remove the direct-line-of-sight, a T_0 chopper is unnecessary (see also the discussion in 2.3).

3.2 Bandwidth choppers

Neutron bandwidth choppers are required in order to restrict the bandwidth ($\Delta\lambda$) of neutrons traveling in the neutron optics. For a 19 m long instrument running at the source frequency of 60 Hz, $\Delta\lambda$ = 3.5 Å. This instrument requires 3 bandwidth / frame overlap choppers of a disk type.

The relevant parameters are the chopper distance from the moderator, d_{MC}, the chopper disk radius to the beam center, and the chopper rotation frequency. From these physical parameters the chopper open angle (the amount of disk that is free from absorbing material) can be calculated.

The following parameters need to be determined:

Chopper	d_{MC} (m)	Frequency (Hz)	Radius to beam Center (cm)	Open Angle (deg)
Bandwidth 1	TBD	10 – 60	TBD	TBD
Bandwidth 2	TBD	10 – 60	TBD	TBD
Bandwidth 3	TBD	10 – 60	TBD	TBD

Tab. 2: Design parameters for the bandwidth chopper system.

In the open position, the chopper transmission should be 1 for all neutron wavelengths, implying that the open angle is a location where no material from the chopper blade is in the beam path. In the closed position, the neutron beam must be attenuated by the chopper blade by at least a factor of 1000 for neutron wavelengths as short as 1 Å.

Via Monte Carlo simulation, we have determined that we can eliminate all $l < 40$ Å neutrons from adjacent target pulses by employing three bandwidth choppers. Long-wavelength neutrons not absorbed by the choppers will be deflected out of the beam by frame-overlap mirrors. We currently plan to place an array of mirrors between the collimating apertures (see below) angled to the beam so that all $l \geq 40$ Å neutrons are deflected. To eliminate all neutrons with $l \geq 40$ Å and pass all neutrons of $l < 20$ Å and divergence $dq \leq \pm 1^{\circ}$, one can use two 16.7-cm-long Ni-coated Si mirrors, inclined at 3° relative to the channel walls. The operation of the choppers and mirrors is complementary. Jeff Penfold of ISIS has pointed out that at least one chopper may be eliminated if the frame-overlap mirrors are set for a lower cutoff wavelength. Such an arrangement would have clear benefits in reliability and cost and will be evaluated during design of the frame-overlap mirrors.

For optimal performance of the instrument, the first bandwidth chopper should be located as close as possible to the moderator. Shielding requirements determine the minimum distance to be ≈5.5 m. However, there are also limitations because of the Liquids Reflectometer's space requirements. At this distance, the centerlines of the two instruments are separated by less than 1 m. It is anticipated that the two upstream bandwidth choppers will fit into the available space only if the disk diameter is reduced from the standard diameter of 70 cm, which is used in the design of the bandwidth choppers 2 and 3. Spatial interference problems between these downstream choppers of the two reflectometers are not expected. Their individual location is less critical and more space is available due to the divergence of the two beamline centerlines. Sufficient space is also required between the bandwidth choppers of the two instruments in order to fit sufficient shielding to reduce background radiation from choppers (material and thickness TBD).

It is important that the guide system be as continuous as is practical. For this reason, it is desired that the section of guide that must be removed to allow for rotation of the chopper blade be held to a minimum with a goal of 2 cm. In order to minimize the number of aluminum windows along the incident neutron flight path, it is desirable that the choppers share vacuum with the guide system. This implies that the housing of the rotor/absorbing disk assembly form a vacuum connection (probably via bellows) to the guide system. This seal must be such that the chopper assembly can be removed from the beam line without affecting the location of the neighboring guide sections, necessitating realignment.

For maintenance purposes choppers must be reasonably easy to access. Choppers 1 and 2 are located close to the target monolith and will likely require top access, given the shielding geometry in this vicinity. The third chopper will be located far enough from the monolith that access from the side may be feasible.

In order to access the first two choppers, the main beamline shutter must be closed. As a matter of course, such action will also shut down the Liquids Reflectometer beamline. Fortunately, bandwidth chopper systems are very reliable such that the probability of such an event is very low. (The choppers will be continuously monitored by a centralized system. The goal of this system is to predict chopper failures early enough such that disastrous failures will not occur during run cycles of SNS.) Given the likely dose levels in the vicinity of the two close choppers, maintenance during a run cycle may involve shutting down adjacent beam lines during removal and installation of a chopper, putting a premium on the speed with which the process can be done. A design goal of under 2 hours should be set for the time required to remove the necessary shielding and the chopper assembly, with an additional 2 hours allocated to install the chopper and reassemble the shielding.

3.3 Chopper control system

An integrated chopper control system will control the phasing of all SNS neutron choppers relative to the source neutron pulses. Phasing tolerances for the bandwidth choppers are TBD. The instrument user will be able to set desired values for chopper phasing and chopper speed.

4. Detector and Data Acquisition System

4.1 Data acquisition system: general requirements

Neutrons scattered from the sample are counted in the detector system located about 2 m from the sample. The detectors must be capable of achieving a peak counting rate of 1.3 x 10^4 neutrons/sec in each pixel (desired pixel size: 1 mm x 1 mm) and 1.2 x 10^6 neutrons/sec integrated over the whole detector [7]. The detectors must have low gamma sensitivity (TBD) and, because of their close proximity to the sample, be capable of operation in a magnetic field (max. magnetic field: TBD). The detectors must have counting efficiencies that vary by less than 0.1% over the duration of a run cycle (typically 3 weeks of operation) and less than 1% in the course of a year. Desired counting efficiencies are > 80% at a neutron wavelength of 3.3 Å.

For measurements on samples in the region of total reflection or of the direct beam profile a peak counting rate of up to 1.3 x 10^6 neutrons/sec in each pixel (1 mm x 1 mm) is expected and 1.2 x

10^8 integrated over the whole detector (numbers are based on instrument simulations). These numbers significantly exceed currently available technology. Thus, these measurements can only be performed while partially blocking the beam with a suitable material (material and thickness TBD).

Table 3 summarizes the requirement for the detector and the data acquisition system. The "desired" values take into account situations with the highest possible counting rates on the detector, e.g. measurements of the direct beam. The "required" values reflect normal operating conditions. The latter numbers are matched by current technology.

Parameter	**desired**	**required**	**comment**
Spatial pixel area (cm^2)	0.01	0.01	0.020 is state-of-the-art for ^{3}He
Total # of pixels	10,000	10,000	
Minimum time of flight (microsec)	8,640	8,640	1.8 Å, 19 m flight path
Maximum time of flight (microsec)	50,426	50,426	10.5 Å, 19 m flight path
Min. time of flight binning (microsec)	10	10	value based on min. moderator emission time (20 microsec fwhm for 1.8Å)
Max # of time channels	1,667	1,667	
Max instantaneous rate/pixel (cts/sec)	1.3×10^6	1.3×10^4	partial beam absorber necessary
Max total instantaneous rate (cts/sec)	1.2×10^8	1.2×10^6	partial beam absorber necessary
Max time-average rate/pixel (cts/sec)	6.2×10^5	6.2×10^4	partial beam absorber necessary
Max total time-average rate (cts/sec)	5.9×10^7	5×10^5	partial beam absorber necessary
Minimum time per data set (sec) *	1	1	
Typical time per data set (sec) *	60	60	
Total # of channels per data set *	1.5×10^7	1.5×10^7	
Typical # of channels per data set *	7×10^6	7×10^6	
Total # of counts per data set *	3.5×10^9	3.5×10^7	

Tab. 3: Desired and required parameters for the SNS Magnetism Reflectometer

When reviewing currently available detector technologies it seems that only ^{3}He type detectors can fulfill the specified requirements.

Furthermore, the detector system must have the following features (all currently under development within SNS shared design activities):
i) an integrated time-of-flight module that determines the neutron arrival time on the detector to better than 1-2 µsec (The error in the time-of-flight should be much less than the time uncertainty introduced by the moderator (about 20 µsec for 1.8 Å neutrons) or by different travel paths of the neutrons through the instrument.)
ii) a fast on-line detector data visualization system
iii) a fast connection to the general SNS data acquisition system

As is schematically shown in Fig. 4, the detector system will be mounted (together with spin flipper and spin analyzer) on an optical bench inside the detector shielding box (see also section 7.2). The angular resolution of the detector can be varied by changing the sample to detector distance. This can be achieved by moving (manually or motorized) the detector along the optical bench. The shielding box will be filled with He gas (ambient pressure) in order to reduce intensity losses due to air-scattering.

4.2 Two-dimensional ^{3}He detector

In view of the different measurement geometries for reflectometry and in-plane diffraction (see also section 1) position sensitive detection of neutrons with a minimum resolution of 1 mm x 1 mm is desirable. At a typical distance of 2 m between sample and detector, this corresponds to 3/100 deg. angular resolution which matches typical angular resolutions of the primary instrument side. In order to completely cover the available signal for large wavelengths up to 10 Å (at this wavelength the transported divergence is in the order of 5 deg., see Fig. 10), the approximate detector area will be 200 mm x 200 mm or larger.

Other applications of the area detector include measurements of off-specular signals, general background determination and measurements of the incident beam profile. For the latter case and also for other high count-rate applications, it is planned to move a partially-absorbing material into the beam in order to reduce the intensity to reasonable levels (see also section 4.). Material and location of the absorber: TBD

4.3 ^{3}He pencil detector

Some additional ^{3}He pencil detectors will be required for two reasons: First, such detectors can be used instead of the ^{3}He area detector during high count-rate experiments. Second, ^{3}He area detectors are technically delicate and usually require more maintenance. It can be foreseen that the ^{3}He area detector will require periodic downtime for maintenance and repair during which the more robust pencil detectors will be used.

5. Polarization Handling

Fig. 11 shows schematically the spin-handling system of the instrument. On the primary instrument side it consists of a polarizer system and a spin flipper. On the secondary side of the instrument the scattered radiation will be analyzed by a combination of spin flipper and focusing stacked supermirror system.

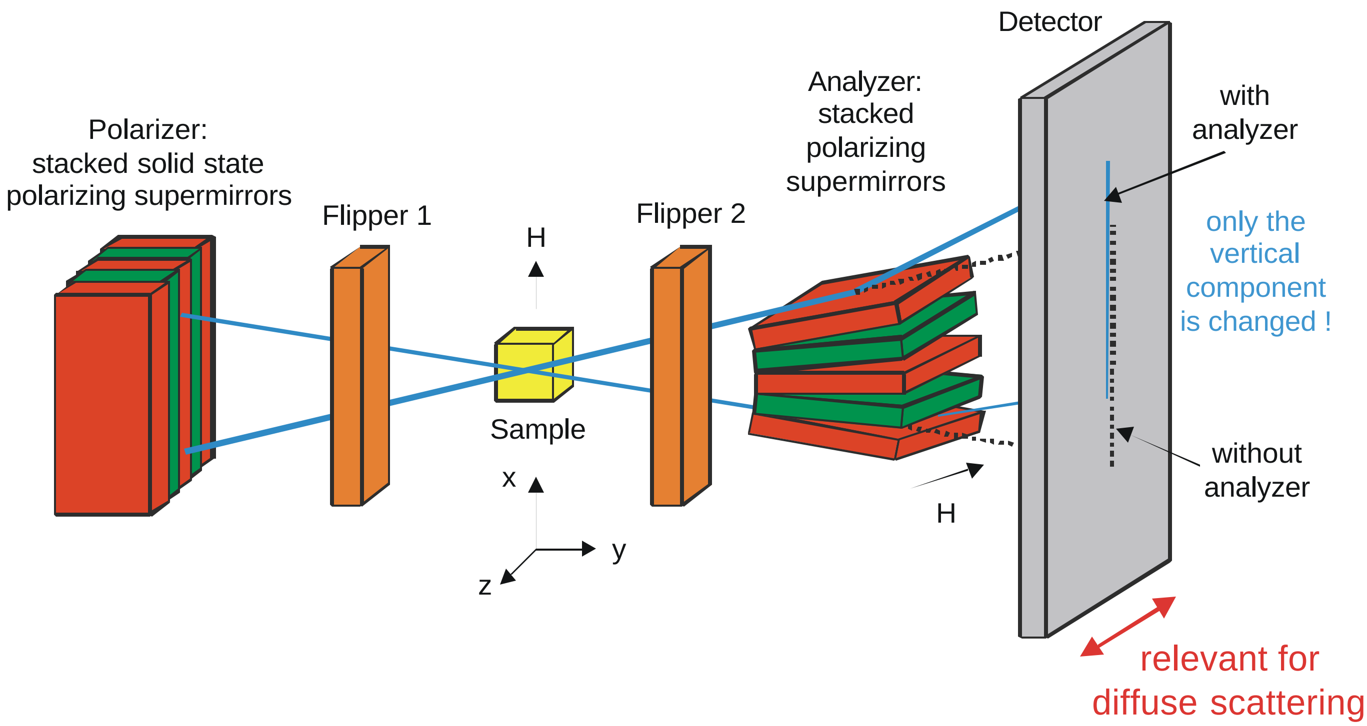

Fig. 11: Spin-handling system of the Magnetism Reflectometer.

5.1 Polarizing optics

In order to polarize the neutron beam, the primary instrument side will be equipped with a curved system of stacked polarizing supermirrors (see Fig. 11). Such systems have been successful to handle the desired high angular divergence (>1 deg., even for small wavelengths).

It has not been decided yet if a conventional system with open channels will be employed (similar to the systems that are for example in use at NIST [8]), or if a "stacked solid state polarizer" system will be used. The latter system was recently developed by the optics group at HMI Berlin [9]. It uses single or double side coated very thin Si wafers (0.25 mm or even less) in transmission or reflection geometry. Compared to a conventional bender it has the following advantages: very compact design (<10 cm), better polarization, inherently broad wavelength band, lower critical angle, higher neutron transmission and higher divergence transmission.

5.2 Analyzing optics

Fig. 12 summarizes the working principle of a stacked focusing supermirror analyzer system (see also Fig. 11). The key feature of this system is that the individual supermirrors are turned in their orientation by 90 deg. relative to the orientation of the polarizing mirrors and the sample surface. Such an arrangement will result only in a vertical offset of the scattered beam. It does not deflect the beam in the horizontal direction, which is relevant for detection of off-specular scattering. Thus, this system will be very useful for distinguishing specular from diffuse scattering. The other main advantage of such a system is its large angular acceptance. As can be seen in Fig. 12 (upper part) neutrons that are scattered non-specularly strike the analyzer with the same angle as specularly reflected neutrons. This is in strong contrast to conventional mirror analyzers, which suffer from very limited angular acceptance.

The lower part of Fig. 12 shows the different signal regions on the area detector (specularly reflected neutrons, off-specular reflected neutrons, and neutrons that are transmitted through the sample) with and without introduction of the analyzer system.

Polarized ^{3}He spin filter technology based on the reaction ^{3}He$\uparrow$ + n$\downarrow$ => ^{4}He* => ^{1}H + ^{3}H has been improved a lot over the recent years [10].
However, there are still some difficulties that hinder the implementation of this technique as the definitive standard neutron spin analyzer. Specific drawbacks are:
i) Achieving and maintaining high and uniform ^{3}He polarization (> 50%) is difficult.
ii) A high beam polarization can be achieved only with modest transmission (example: P = 84%, T = 12% at λ = 4.5 Å).
iii) ^{3}He polarization decays exponentially (at least when using the European approach, current time constants: about 82 h).

In view of the planned experiments (see 1.1 - 1.4) the performance of the reflectometer would not gain much from the main advantage of the ^{3}He technique, namely that the spin analyzing capability is not depending on the scattering angle. There is no demand for analyzing more angular range than a few degrees at the same time. Such performance can easily be reached by supermirror based analyzer systems which have higher transmission and better spin analyzing capability.
The Magnetism Reflectometer will use polarized ^{3}He spin filter technology only if the above discussed problems can be sufficiently minimized, or if offsetting advantages are seen.

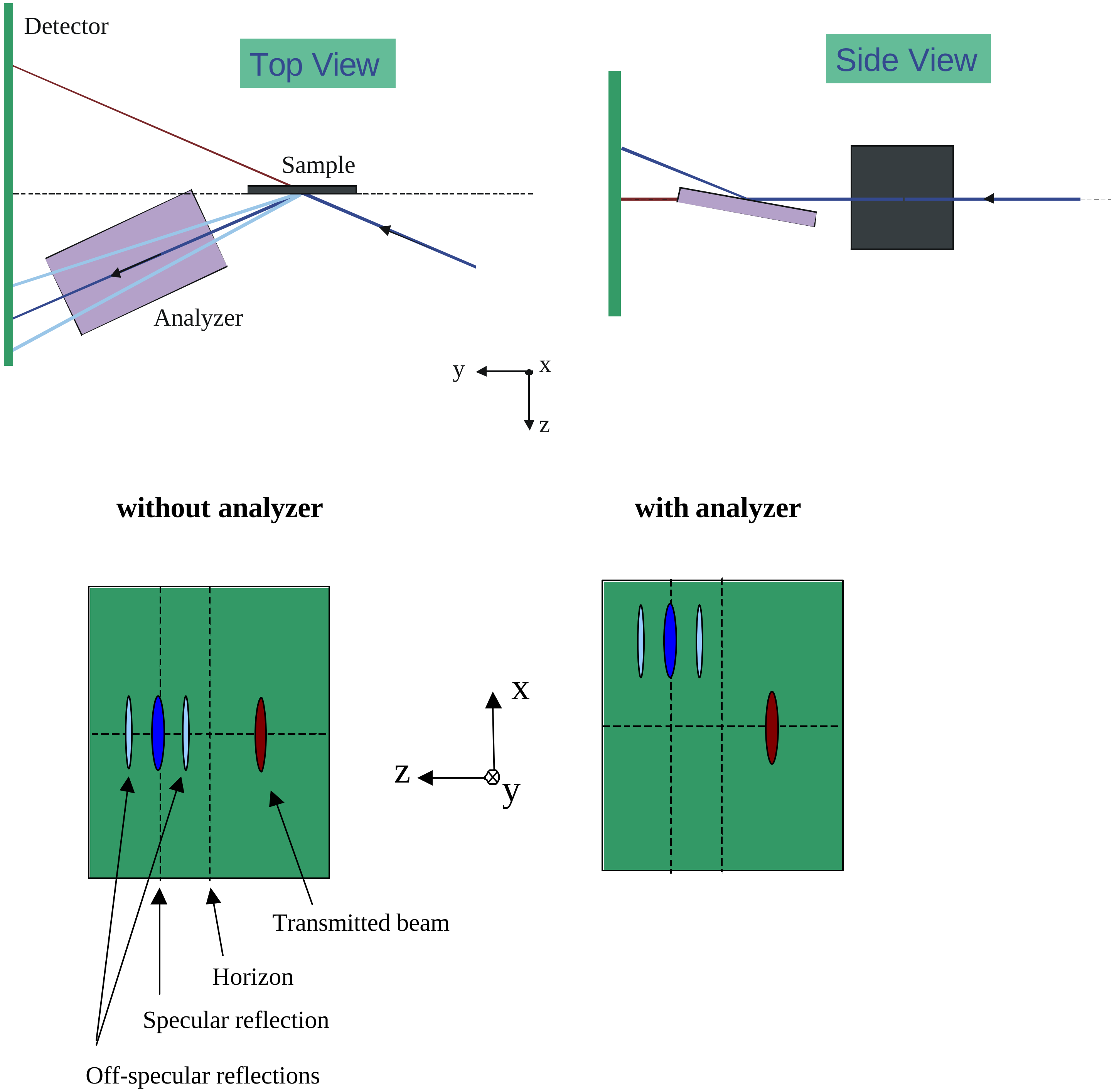

Fig. 12:
Upper part: Schematic representation of the geometrical arrangement of the analyzing optics.
Lower part: Schematic representation of the scattering pattern on the area detector without (left) and with (right) analyzer.

5.3 Spin flippers

A spin flipper is used for reversing the neutron spin direction after the beam has been polarized initially. A second spin flipper will be located immediately in front of the spin analyzer system on the secondary side of the instrument. Both flippers must be able to handle wide bandwidth (it is planned that at least the first 3 frames will be used for data collection, which corresponds to a wavelength band of 1.8 Å to 10.5 Å). The efficiency should be better than 99.9% for all wavelengths. This value should be reached over the full 25 mm x 25 mm area of the beam at the incident side of the instrument and, due to planned off-specular measurements, over an even wider area at the secondary side. It seems that a design based on radio frequency flipping fields and a gradient magnetic field configuration fulfills these requirements [11].

Fig. 13 shows the radio frequency (RF) flipper mounted between the aperture systems on the incident optical bench of the Magnetism Reflectometer. In the figure, the sample is located between the coils of a superconducting magnet. The detector assembly is shown on the left side. One should note that for high-field applications the fringe field might interfere with the RF flipper so that the distance between flipper and magnet will need to be optimized.

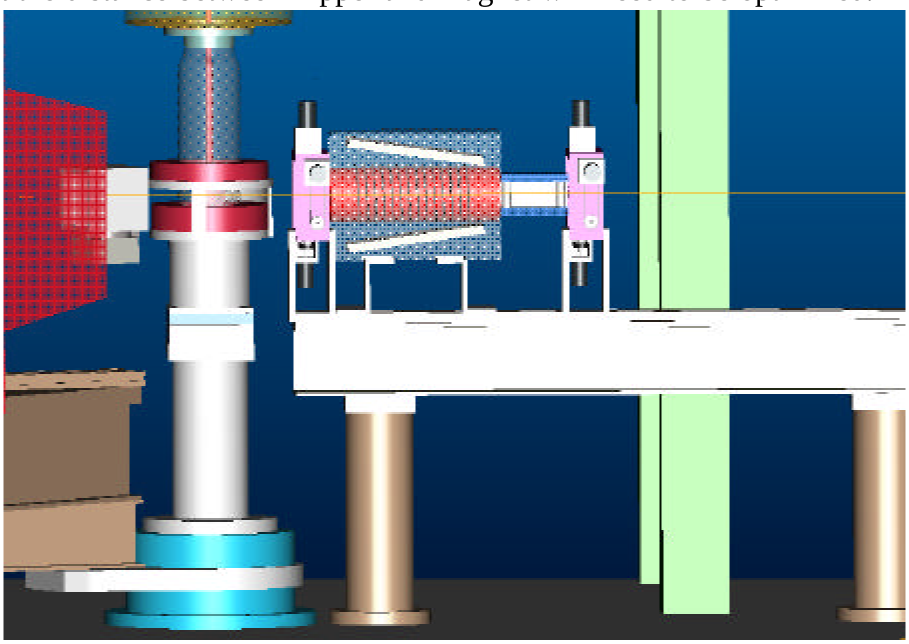

Fig. 13: Incident beam polarizing optics (spin flipper and polarizer mounted between aperture systems).

5.4 Guide field setup

A neutron spin guide field is required between the polarizer and the analyzer systems in order to keep the beam polarized. Virtually no neutron spin precession can be allowed to occur due to the earth's field or magnetic stray fields of instrument components. Static fields on the order of several tens of Gauss are usually sufficient to serve this purpose (see also section 5.5).

5.5 Interference with sample magnets

The instrument's polarizing/analyzing system will be designed such that very strong magnetic fields can be used at the sample position. For certain experiments, superconducting magnets with fields > 15 Tesla are desirable. In contrast to electromagnets, no yoke is used in superconducting magnets. Thus, these magnets often have a strong return field that might interact with the magnetic field configurations of polarizer, analyzer, spin flippers and, of course, the guide fields. Due to these reasons, it is desirable to set up the polarized optics components not in the immediate vicinity of the sample position. When extremely large sample fields are used it might be required to use additional electrically driven guide field arrangements besides the normal static guide fields.

5.6 Drabkin TOF energy filter

As described above, the instrument will be located on a coupled liquid hydrogen moderator, which delivers an intense cold neutron flux. In order to gain even more intensity, a further tradeoff between emission time and intensity could be made (see discussion in section 2.1). Feasibility studies are currently under way. However, a high-intensity moderator would introduce a relatively large time-uncertainty and a corresponding wavelength-uncertainty into the measurements. For most applications this feature can be tolerated. The main disadvantage of such a moderator is that the resulting loss in resolution prevents reflectivity measurements on layers with film thickness above ≈3000 Å. In order to be able to resolve diffraction features ("Kiessig fringes") of films in this thickness region, one needs to introduce some mechanism that artificially creates smaller moderator emission times. Such a device will be particularly useful if it could cut the long moderator emission "tails" that are characteristic for a coupled moderator.

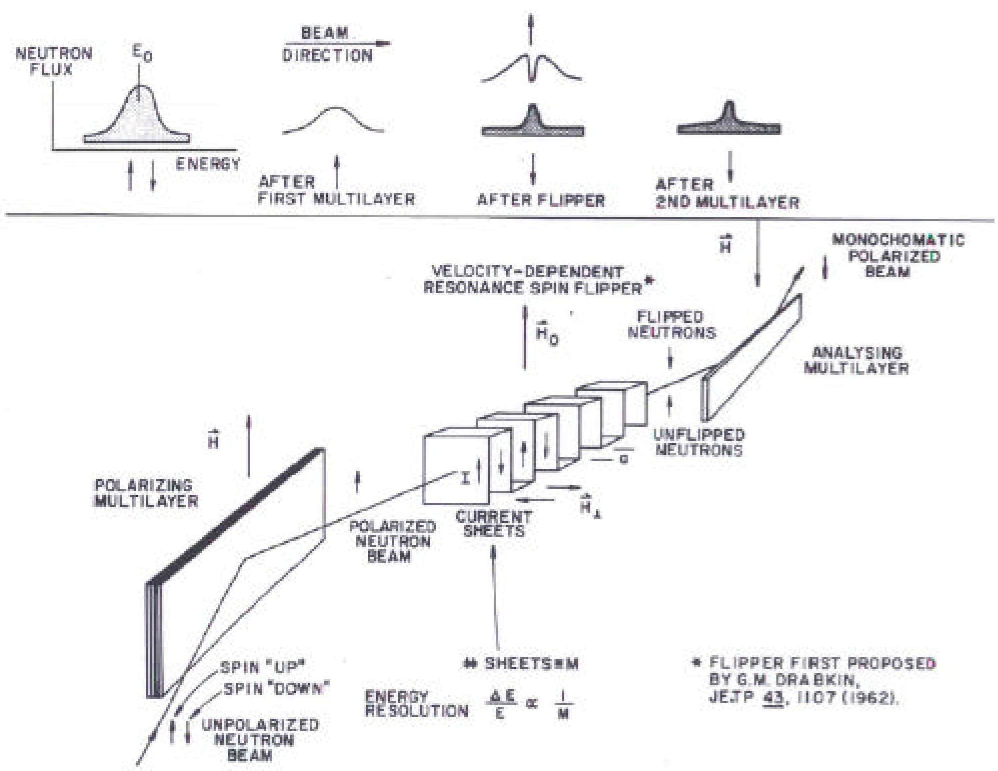

Fig. 14: Basic principle of the Drabkin energy filter.

As early as 1962, Drabkin proposed an energy-filtering device based on the spatial spin-resonance effect [12]. It allows transmission through the device for only a selected neutron bandwidth range and rejects practically all other neutrons. The basic function is sketched in Fig. 14.

After an initial supermirror that is used to polarize the beam, the neutrons travel through a magnetic resonator. In this case the resonator consists of a periodically folded plate current foil and a guide field assembly. Depending on the current that is driven through the current sheet, the number of plate folds and the strength of the guide field, a certain wavelength band will experience a resonance condition resulting in a spin-flip. These neutrons are separated from those neutrons that are not spin-flipped by another supermirror.

The Drabkin energy filter has been used successfully in Russia and also at Brookhaven and NIST by L. Passell and C. Majkrzak. These groups have used the concept in a static way as a neutron monochromator with selectable wavelength resolution.

The Drabkin energy filter concept can also be applied to time-of-flight experiments with only minor changes. The basic idea is to create a resonance condition such that only neutrons having two selected parameter values (in time and in wavelength) will be transmitted. Neutrons that do not fulfill both conditions, for example those neutrons from the moderator tail, will not be reflected by the second mirror and later absorbed. For TOF applications, the magnetic fields must be drifted in time such that there is a correct resonance condition when each individual neutron wavelength will nominally pass through the device. After transmission through the energy filter, the wavelength-time relation will be much sharper than before, which results in a higher Q-resolution in the experiments. Another useful application of the device is that it will filter out the steady background of delayed neutrons, which are constantly emitted from the target or from activated shielding. Even though the expected number of the delayed neutrons is relatively small (delayed neutrons from the target represent only a fraction of about 10^{-4} from the total neutron emission) they can be disturbing in particular experiments.

Preliminary calculations have shown the feasibility to apply the Drabkin energy filter approach to time-of-flight instruments (A. Parizzi, F. Klose). It may be possible to directly use a prototype of such a device that had been built for NIST (C. Majkrzak, L. Passell) with only minor modifications. Current state-of-the-art power supplies easily fulfill the requirements for operating the device. Fig. 15 shows the NIST device before shipment to Argonne.

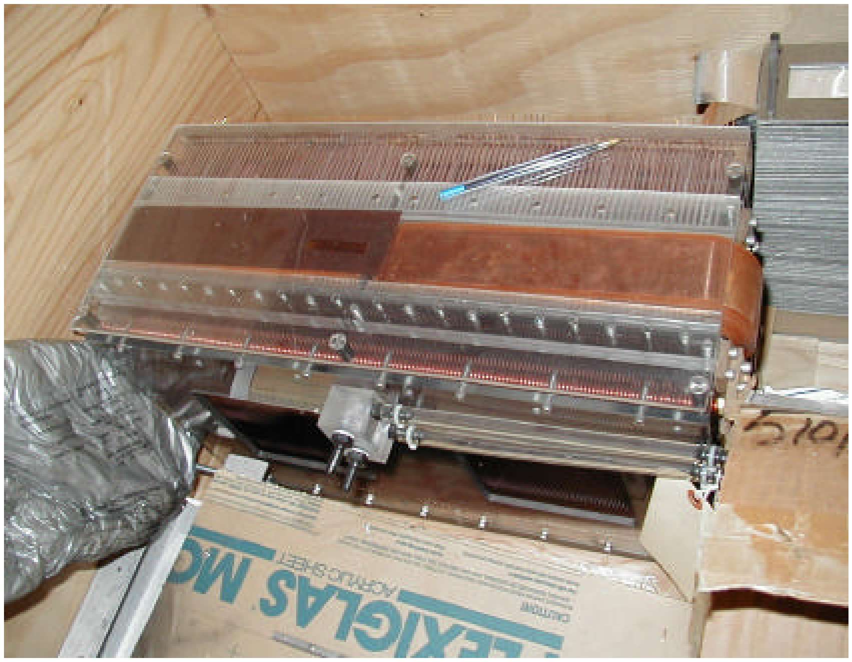

Fig. 15: Prototype of the Drabkin energy filter developed by C. Majkrzak and L. Passell.

6. Sample Environment

The sample environment serves two main purposes: First, the sample must be supported physically and oriented spatially with very high precision. Second, the sample environment must provide a variety of external physical or chemical fields/conditions to the sample (temperature, magnetic field, partial gas pressures etc.). Most likely, one will not succeed to cover all demands with a single sample environment setup. However, the design tries to include those features in a "standard" unit that will be used for the majority of experiments. Exceeding requirements will be met by specialized equipment, which might be shared between a number of SNS instruments or designed solely for the Magnetism Reflectometer. An example for the first case would be a cryostat that will provide extremely high magnetic fields (> 15 T), while the in-situ UHV chamber (see below) is an example for the latter case.

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6.1 Goniometer

The basic purpose of the goniometer is to support the sample chamber and to provide an accurate alignment of the sample relative to the neutron beam. The planned reflectometry and diffraction experiments typically require an angular precision of a few 1/1000 deg.

The required angular and linear movements are shown in Fig. 16. For both vertical and horizontal sample surface measurement geometries, a ω-movement and a height adjustment of the sample are necessary. Note that different sample tilt axes are required for the two setups. In the vertical surface orientation, one needs to control the sample tilt angle α (perpendicular to the neutron beam axis and scattering vector) very precisely. For the horizontal scattering experiments, one needs to control the sample tilt angle β precisely, which determines the angle between the sample surface and the incident neutron beam.

An appropriate feedback system (e.g. optical encoders) is required for all motion axes to confirm angular or linear positioning of the goniometer.

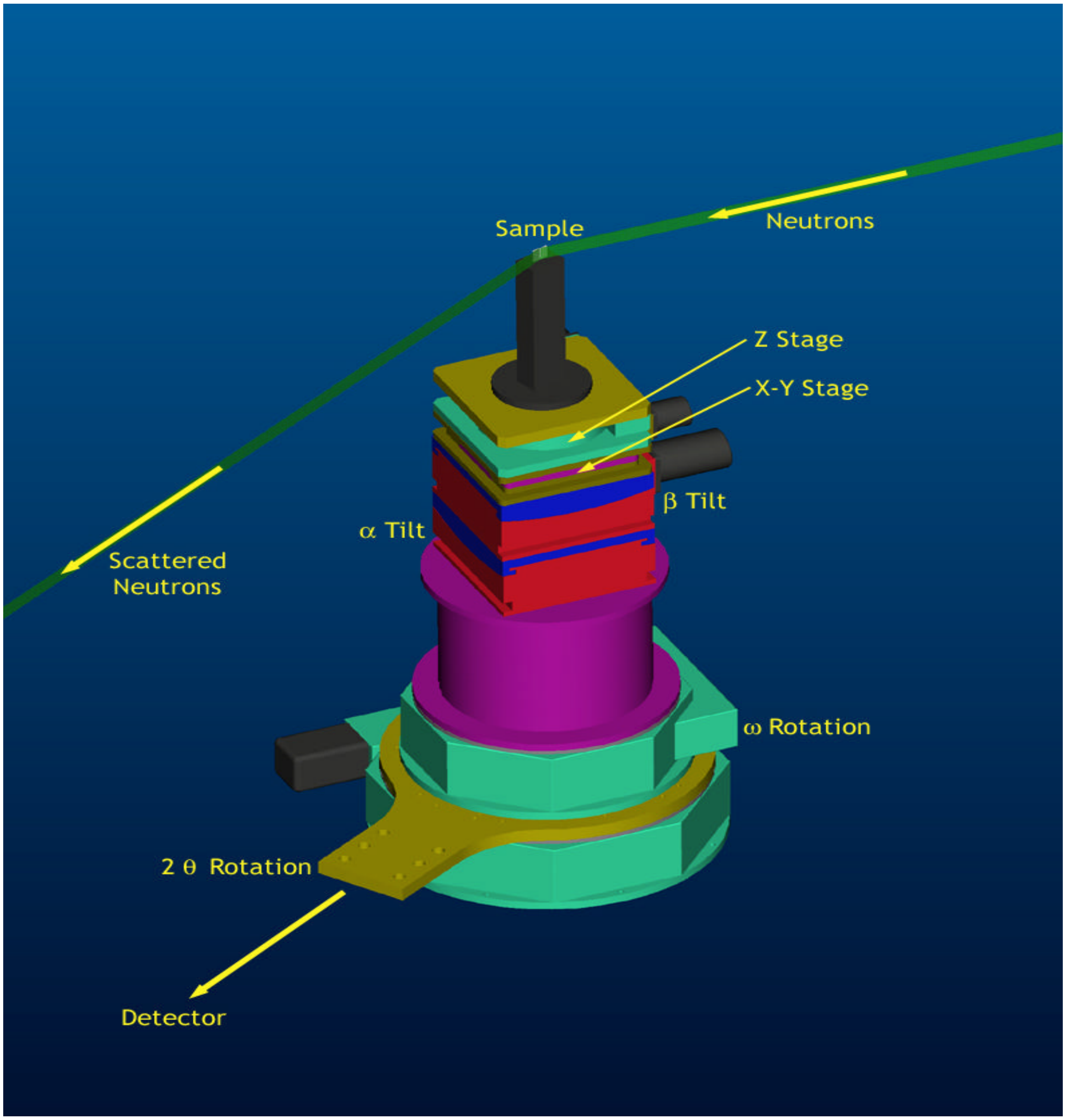


Fig. 16: Required angular and linear movements of the goniometer.
(Shown is a sample in the vertical sample surface diffraction setup. The sample is supported by a generic support. For clarity, sample chamber, magnet and cryostat are suppressed.)

- w rotation
precision: 1/1000 deg.
range: - 10 deg. => 100 deg. (relative to the neutron beam axis)

- Sample tilt a
precision: 1/1000 deg.
range: +/- 5 deg.

- Sample tilt b
precision: 1/1000 deg.
range: +/- 5 deg.

- Eulerian cradle movement (optional concept for non-normal scattering directions)
precision: 1/1000 deg.
range: - 10 deg. => 100 deg. (relative neutron beam axis)

Linear motions
Linear motions along all three dimensions are required for precise adjustment of the goniometer itself and of the sample position:

- X-axis (horizontal movement, along the nominal beam axis)
precision: 1/100 mm
range: +/- 20 mm

- Y-axis (horizontal movement, perpendicular to the neutron beam)
precision: 1/100 mm
range: +/- 20 mm

- Z-axis (vertical movement, aligns sample height relative to beam nominal axis)
precision: 1/100 mm
range: +/- 20 mm

- Max. load on goniometer: > 800 kg (should be able to support high-field magnet or dilution fridge cryostat)

6.2 Sample chamber
The goniometer will be equipped with a sample chamber that will be appropriate for the majority of experiments. The design has to be such that this chamber will fit inside the bore (or the pole shoes) of the standard sample magnet (most likely, the standard magnet system will be a three-dimensional superconducting unit). For convenience reasons, the same sample mount should also be used for samples that do not require a vacuum environment. The sample chamber will be located in the center of the diffractometer and needs to be properly attached to the goniometer.

The time required to evacuate this chamber from atmosphere to a base pressure of 10^{-6} Torr must be less than 5 minutes. The sample chamber vacuum system will therefore include an appropriately sized turbo pump. For certain types of experiments this chamber needs to be evacuated down to a minimum pressure of some 10^{-8} Torr. This requires that the walls of the chamber should be bakeable to T < 150 deg. Celsius.

Because of the requirement to allow for large magnetic fields at the sample, the scattering chamber should be constructed of a non-magnetic material (most likely aluminum). The sample chamber will have thinned windows in paths of the incident, transmitted, and scattered neutrons. This chamber will have external dimensions of TBD, large enough to contain a heating/cooling stage (desired range: 10 K - 1100 K) and a rigid sample mount. A closed-cycle refrigeration system is the preferred cooling mechanism.
Certain types of experiments require the presence of a controlled gas atmosphere (for example N_2, H_2 etc.). Thus, external gas supply lines have to be provided.

For certain experiments it would be desirable to measure magnetic hysteresis loops on-line by means of the magneto optical Kerr effect technique (MOKE). The use of this technique should be made possible by equipping the sample chamber with light-transparent windows.

Standard sample chamber requirements:

Sample size:	up to 25 mm x 25 mm
Temperature range:	10 K - 1100 K
Vacuum:	< 10^{-8} Torr

6.3 Sample magnet and temperature combinations

The IAT has demanded a large variety of temperature and magnetic field combinations (3.5 K – 1070 K, XYZ field capability up to 1T, high-field capability up to 17 T in vertical direction). However, one cannot practically meet such expectations with just a single device. Therefore, two temperature/magnet combinations are proposed:

- XYZ superconducting magnet and standard sample chamber

The standard sample chamber (see 6.2) will be used in conjunction with the XYZ magnet. Two field-axes of this magnet will be used to rotate the magnetization vector into any desired direction within the sample plane. For most samples only low/medium fields on the order of 0.4 Tesla are required. However, the third field-axis should be capable of magnetizing a sample along its surface normal direction. For an iron film, one would require 2.2 Tesla. The design of an XYZ prototype magnet is currently under way in a collaboration between G.P. Felcher / ANL and the company Janis Research / Wilmington.

XYZ superconducting magnet requirements:

Max. field strength along X,Y axis:	0.4 Tesla
Max. field strength along Z axis:	2.2 Tesla
Field homogeneity:	better than 1-2 % over a volume of $(25\ \text{mm})^3$

- Low temperature cryostat with high-field superconducting magnet

Very high magnetic fields can only be achieved by using specialized cryostats. Such equipment is expensive and, since it is required for only a small number of reflectometry/diffraction experiments, should be shared between several SNS beam lines. A system that reaches 17 Tesla was built by Oxford Instruments and serves as an example here. A quite similar design can be expected for the actual high-field cryostat that will the used at the Magnetism Reflectometer.

Example of a high-field magnet system:

Manufacturer:	Oxford Instruments, Oxford, GB
Temperature Range:	300 K - 1.5 K
(with Dilution Insert:	- 100 mK)
Sample Diameter:	< 15 mm
Split:	20 mm
Angle:	±2°
Weight:	700 kg (incl. cooling liquids)
LN-Refill Interval:	3 days
LHe-Refill Interval:	5 days
Magnetic Field	
(at 4.2 K):	13 T (symmetric)
(at 2.5 K):	15 T (symmetric)

The magnetic stray-field on the lower wall plate amounts to 5 kG (1 kG at 1 m distance)

Horizontal Access: total view 335 deg. (25 deg. dead angle)

Total Thickness of AL-Screens and Al-Rings in Split: circa 2 x 40 mm

Thermometry Sensors: Cernox®

Fig. 17 and 18 show a cross section of the cryostat and details of the spacer ring arrangements.

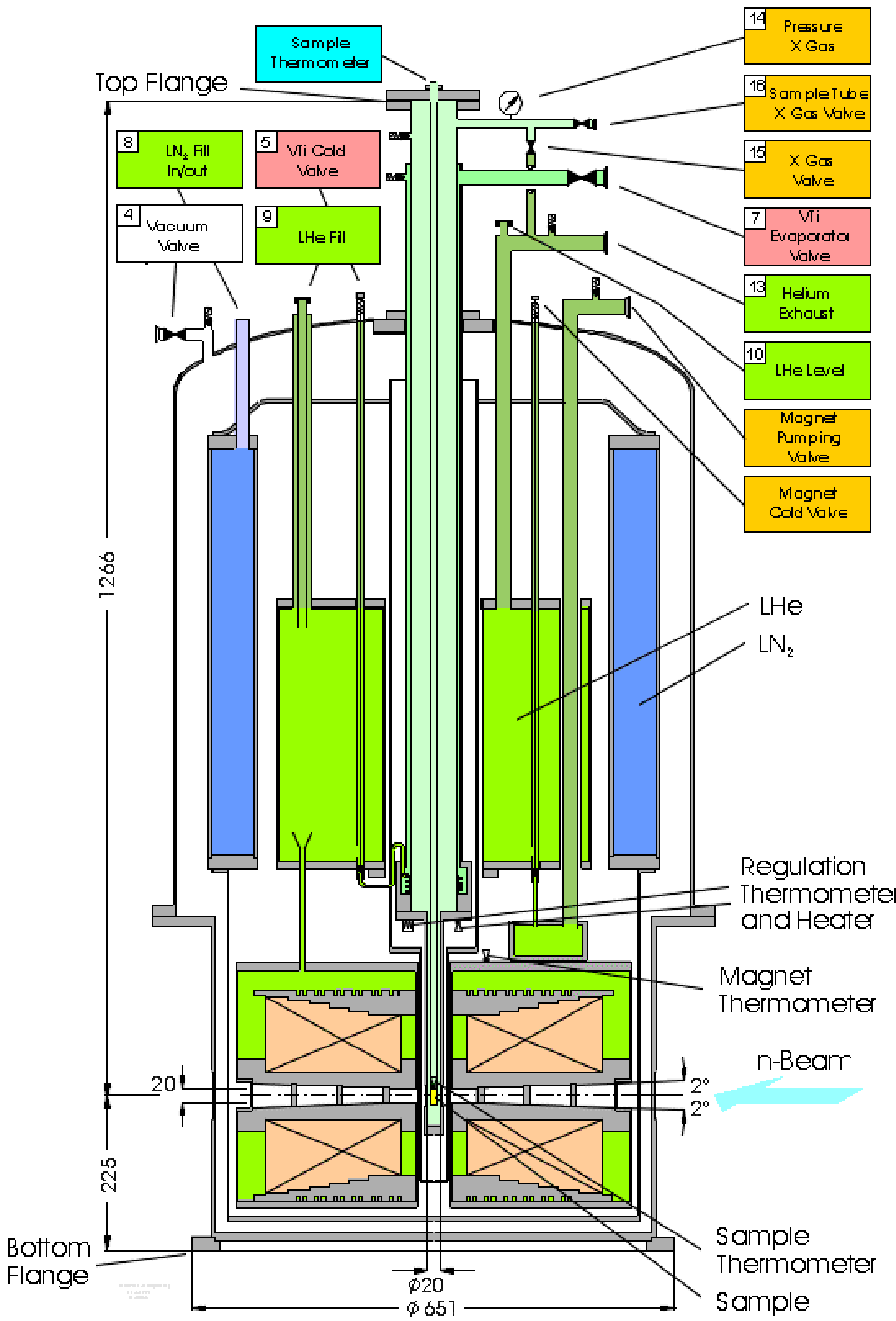


Fig. 17: Cross section through a typical high-field magnet system (see text).

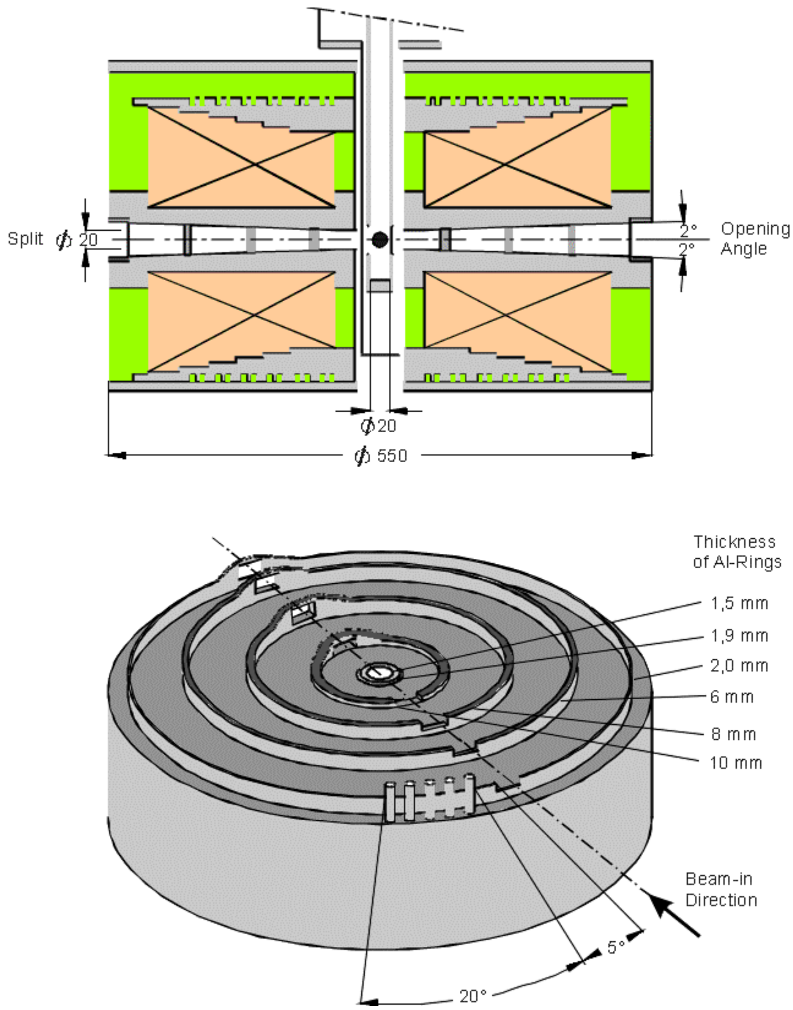


Fig. 18: Spacer ring arrangement of a typical high-field magnet system (see text).

General drawbacks of a high-field cryostat system are:
- The sample can be no larger than 15 mm diameter (the split is only 20 mm).
- The vertical angular divergence is limited to +/- 2 deg. due to the limited open angle of the magnet.
- The incoming/diffracted beam has to pass through a number of Al rings (in total: 40 mm), which leads to beam absorption and small-angle scattering.

It should be mentioned that the above stated drawbacks relax for magnet systems that do not require extreme high fields. A comprehensive overview about specifications of cryostat/magnet systems that are in use at the Berlin Neutron Scattering Center is provided at:
http://www.hmi.de/bensc/sample-env/home.html

6.4 Ultrahigh vacuum system for in-situ sample preparation

Reflectometry is a surface sensitive method. However, with the neutron flux that is available at today's state-of-the-art instruments, it is not possible to resolve diffraction features of magnetic

surfaces or monolayer films within a reasonable data collection time. Complete reflectivity scans down to values where those features can be observed (typically in the 10^{-8} region) take on the order of 12-24 hours. Such duration of time normally prevents successful studies of uncovered surfaces or monolayer films with the reflectometry technique, simply due to the fact that the surfaces do not stay clean long enough even in a vacuum in the 10^{-11} Torr region.
What has been done until now for the case of monolayer films is to use cover layers that artificially enhance the contrast [13]. Thus, the measured signals are due to an interference effect between the monolayer film and the cover layer but they do not represent a diffraction feature characteristic to the individual monolayer film or surface feature. The need for cover layers decreases the number of magnetic monolayer materials that can be investigated to a handful of film / cover layer systems. In the vast majority of other cases, the cover layer will change the properties of the magnetic monolayer film due to electronic interactions at the interface between the materials. To my knowledge, no successful neutron reflectometry experiments on uncovered magnetic surfaces have ever been reported, except one experiment carried out at HMI Berlin [14]. The purpose of this experiment was to demonstrate the feasibility of the in-situ neutron reflectometry technique. Unfortunately, the flux of the Berlin reactor is low and therefore the system is not used often for in-situ experiments.

At the SNS Magnetism Reflectometer, the available neutron flux will allow complete reflectivity scans down to the 10^{-8} region on a time scale of minutes. Even 10^{-10} reflectivities can be measured in a few hours. This fact strongly suggests that the Magnetism Reflectometer should be equipped with a dedicated in-situ UHV sample preparation chamber. There is a clear opportunity for new science that should not be missed !

Fig. 19 shows schematically the UHV system proposed to be set up at the Magnetism Reflectometer beamline for in-situ experiments. It is designed such that polarized reflectivity, diffraction and grazing-incidence diffraction experiments (within the sample plane) are possible. The whole system will be mounted on a platform. When the system will be used for experiments this whole platform (with all components of the UHV system) will be moved to a position above the goniometer by a suitable crane or other device. Since all parts of the system will stay together the entire time, the setup time of the system will be in the order of 1 hour.

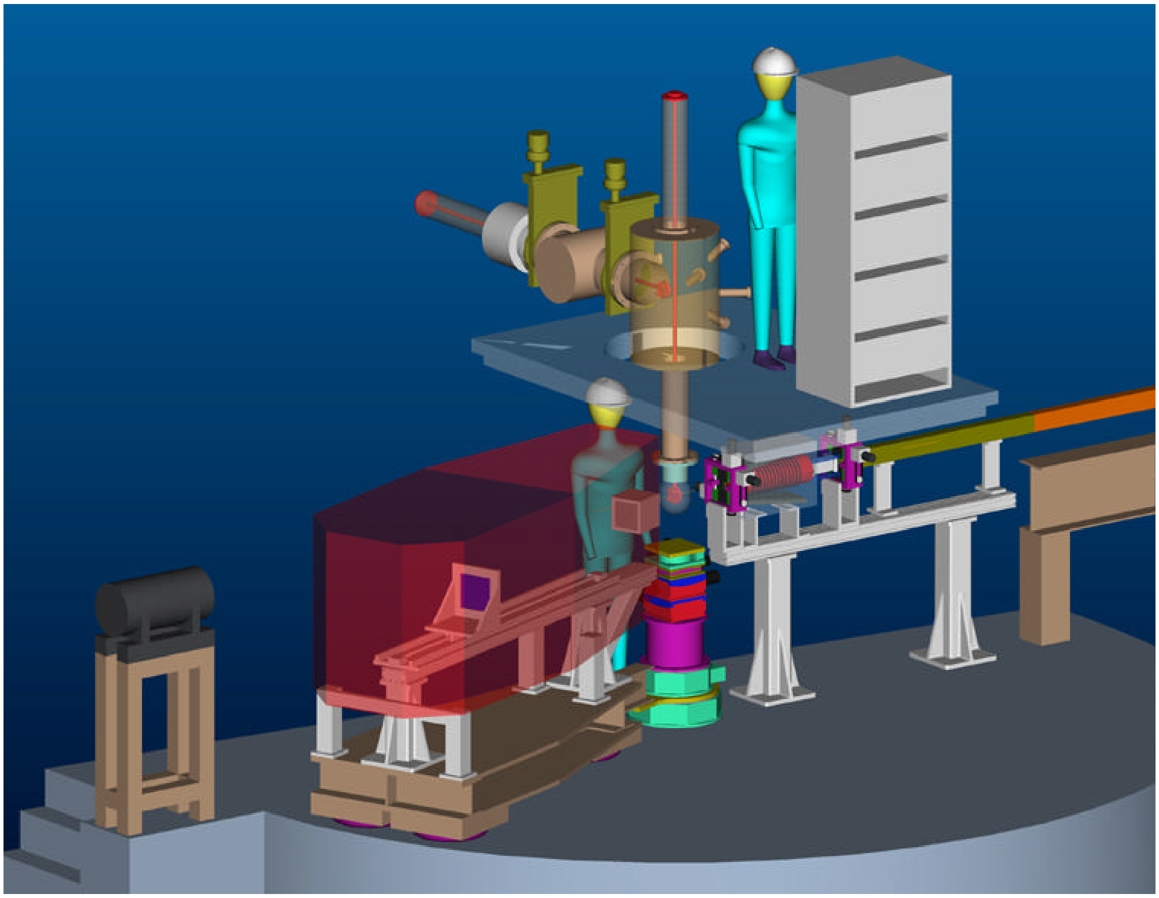


Fig. 19: UHV system for in-situ polarized reflectometry experiments on ultrathin magnetic films (for clarity reasons the sample magnet is suppressed).

The substrates will be introduced via a load lock system. Depending on the substrate/material combination, the monolayer film will be either produced by electron beam evaporation (main chamber) or by ion-beam sputtering (separate chamber). The main chamber will contain suitable equipment for chemical/structural characterization of surfaces and films (LEED, RHEED, mass spectrometer, Auger spectrometer etc., see below for details). The sample will be brought into position for the neutron measurements by using a transfer system, also called a translator. This translator also contains the sample holder system (with heating/cooling capability) and provides all necessary angular movements for the diffraction experiments. During the scattering experiments the sample will be located inside a quartz glass tube that is sufficiently transparent for neutrons. During initial alignment of the sample platform the quartz tube will be moved into the center of the XYZ magnet, such that the sample is centered relative to the neutron beam. The goniometer will be used for supporting the magnet.

Fig. 20 shows schematically the details of the UHV system.

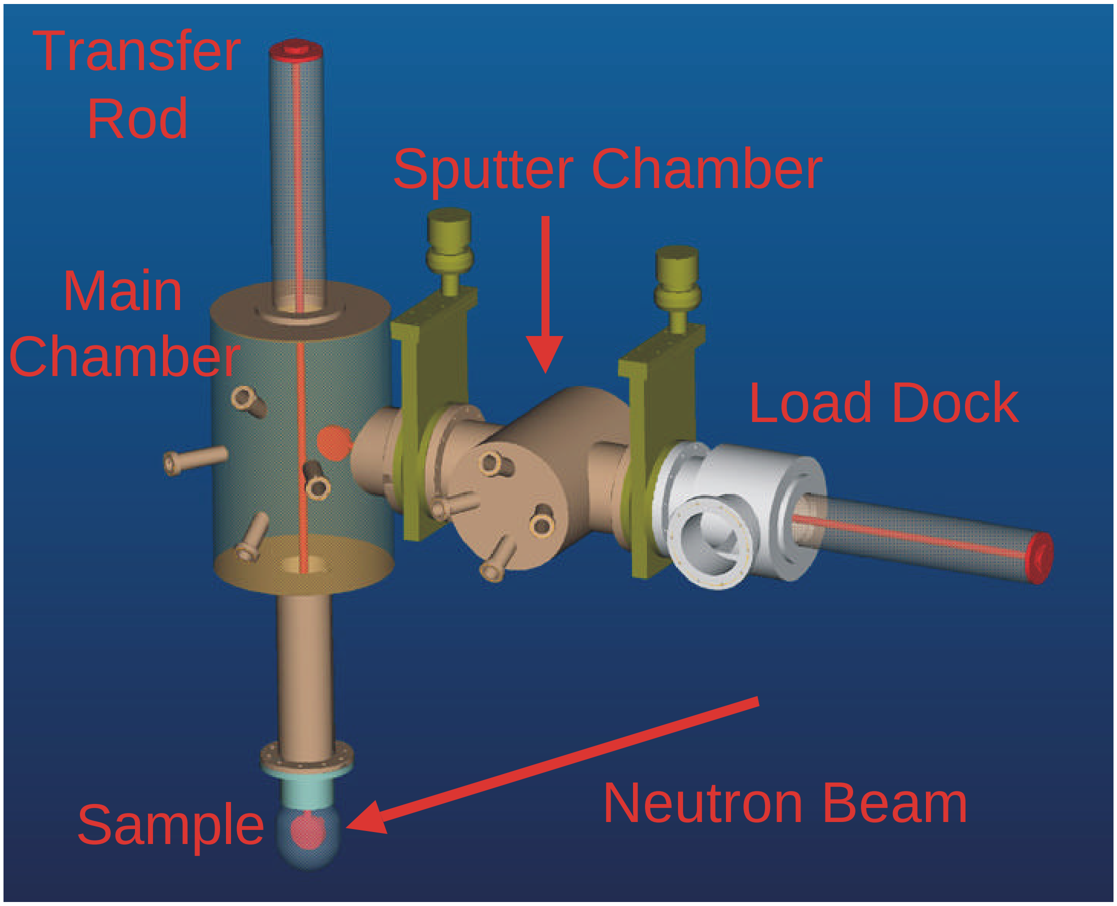


Fig. 20: Schematic layout of the UHV system.

- Specifications for the UHV sample environment:
Main analysis chamber:
- 1 LEED/Auger system for chemical/structural surface analysis
- 1 RHEED system for grazing-incidence electron diffraction and analysis of monolayer growth
- 1 MOKE system for fast hysteresis measurements
- 1 Quadrupole mass spectrometer (100 amu)
- 1 Sputter gun for sample cleaning
- 2 Thin-film thickness measurement system (based on quartz crystal microbalance)
- 2 High-temperature effusion cell systems
- 2 E-beam evaporation systems for rod-evaporation
- 1 Sample manipulator (sample size 25 mm x 25 mm, temperature range: 100 K - 1200 K, sample rotation and translation capabilities, z-axis translation must be about 1 m for transfer of sample from sputter/load lock chamber into neutron beam position)
- 1 Neutron scattering chamber (Pyrex or quartz glass)
- 1 Ion-getter pump system with integrated Ti sublimation pump
- 1 Vacuum pressure measurement system

Vacuum requirement: 5×10^{-11} mbar

Sputter chamber:
- 1 Sputter target station (about 4 targets)
- 1 Ion beam source for sample preparation via ion beam sputtering technique
- 1 Sample holder (with rotation possibility)
- 1 Sample transfer stick
- 1 Turbo molecular pump (500 l/s)
- 1 Vacuum pressure measurement system

Vacuum requirement: 5 x 10^{-10} mbar

Load lock chamber:
- 1 Vacuum pressure measurement system
- 1 Turbo molecular pump (340 l/s)
- 1 Loading door
- 1 Sample transfer stick
- 1 Infrared heating lamp for water removal

Vacuum requirement: < 1 x 10^{-9} mbar

Also necessary are:
- 1 Stainless steel frame to support the complete system
- 1 Bake out system (< 150 deg. Celsius, incl. controller)
- All required power supplies, electronics and racks.

7. Shielding

7.1 General guide shielding

Dose rates outside the beamline shielding shall satisfy the SNS shielding policy requirements of 0.25 mR/hr on contact. Beamline shielding must also satisfy the seismic stability requirements for personnel protection of Performance Category 1 (PC-1). A major seismic event with a 500-yr recurrence period must not cause the structure to shift or fall in such a way as to cause injury to personnel working in the immediate vicinity.

- Shielding materials and required shielding thickness at various positions

A rough estimate for the required shielding thickness is 1 to 1.4 m in all directions around the beamline. The shielding material will be a combination of steel (major contribution) and other materials such as borated concrete. Calculations are currently under way to determine the most appropriate shielding design. These simulations are based on a realistic geometrical model of the two reflectometry beamlines.

- Transition to reduced shielding

There might be a possibility for a transition to reduced shielding. This concerns the area 2 m after the direct-line-of-sight to the moderator is lost and the beginning of the optical bench in front of the sample.

7.2 Specialized shielding

- Bandwidth chopper cavity

Special shielding blocks have to be fabricated for the immediate area around the bandwidth choppers. A tight fit has to be achieved in order to prevent escape of secondary radiation or scattered neutrons. It is also required that the chopper shielding is easily removable in order to achieve fast chopper maintenance periods. (Materials and design of bandwidth chopper shielding: TBD)

- Sample area shielding and instrument enclosure

Dose rates in the sample area will be sample- and sample environment dependent. Since high-energy neutrons and gammas are already filtered by the bender (see 2.3), no massive shielding will be required in this area. Nevertheless, it cannot be expected that the dose rate in the vicinity of sample and detector will be less than 0.25 mRem/h. Therefore, it is planned to build an instrument enclosure from shielding material.

The enclosure serves three purposes:

i) It prevents scattered neutrons and gammas from leaving the immediate sample / detector area.

ii) It serves as a physical barrier and prevents people from accessing the instrument while the beam is on (see also section 7.4).

iii) It protects the Magnetism Reflectometer's detector from scattered radiation escaping from other beamlines.

It is expected that the top flange of the cryostat will be accessible to personnel while data is being collected (auxiliary shutter in the open position). For this purpose the top shielding plate needs to have an appropriately sized indentation, which might be capped with additional shielding material, if necessary.

Fig. 21 shows a preliminary arrangement of shielding and instrument enclosures. As can be seen, the instrument enclosures are designed in a way that independent access is possible to both instruments.

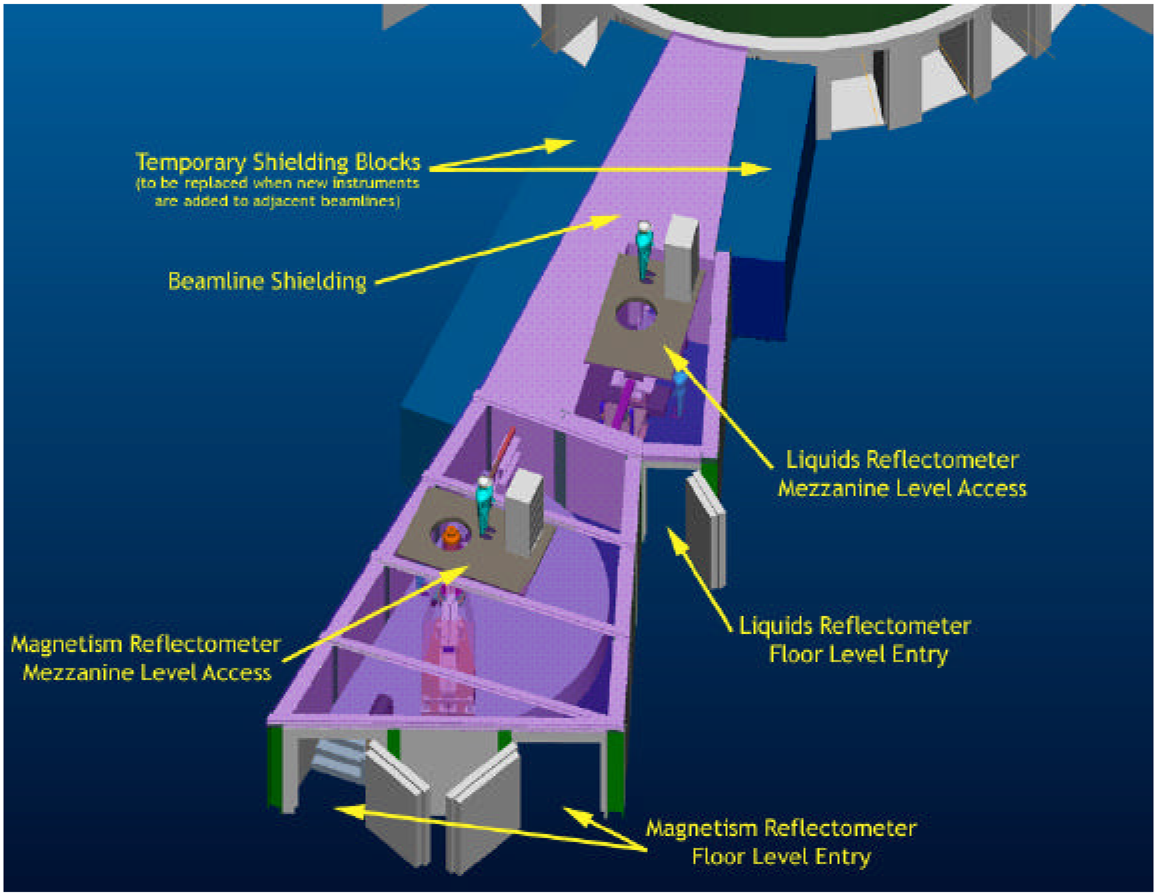


Fig. 21: Preliminary arrangement of shielding and instrument enclosures at the reflectometry beamlines. The shielding blocks that constitute the roof are suppressed for clarity reasons.

- Detector shielding

Achieving low background at the detector area is of high priority. This will be accomplished by surrounding the detector with shielding material (materials and thickness: TBD). The shielding must be sufficient to ensure that only the detector dark count (exact value: TBD) is measured in the absence of a sample with the secondary beam shutter open. This requirement dictates the use of a He-filled or evacuated flight path between the sample table and detector. Due to practical reasons all optical elements on the secondary instrument side will be inside this volume surrounded by the detector shielding. The detector shielding will have a "nose" like shape with the tip of the nose directed towards the sample (see Fig. 5).

- Beam stop

The beam stop will block access to the neutron beam transmitted through the sample. The beam stop will be constructed so as to limit radiation dose rate levels to < 0.25 mR/hr on contact. It will be sufficiently long such that neutrons that scatter from its end have a small likelihood of reentering the scattering chamber or detector.

7.3 Auxiliary shutter

An auxiliary shutter will be installed after the exit of the tapered guide (TBD m from the moderator face). The shutter must be of sufficient thickness and composition to reduce exposure in the beam at the sample position to 2 mrem/hr. Due to the filtering effect of the upstream optics (see section 2.3), only neutrons of wavelength $l > 1\,\text{Å}$ need to be absorbed. It will be interlocked to the sample area access system such that an attempt to remove a sample without first closing this shutter will turn off the beam of protons on target. Its location will be monitored by the SNS Personnel Protection System. Position of this shutter will be clearly indicated by a set(s) of indicator lights visible from inside the instrument enclosure, from inside the instrument control hutch, from the cryostat / UHV system access platform, and from the floor level in the instrument building.

7.4 Safety issues

Only qualified users will have access to areas of the beamline where higher radiation levels than 0.25 mR/hr on contact are expected (close to sample, detector and beamstop). A suitable barrier (shielding and physical barrier) has to be erected to separate these regions from other freely accessible areas inside the SNS experiment hall (see section 7.2). An interlock system will be used to prevent the presence of people in these areas while the auxiliary shutter is open. Should the entrance door be opened by any means or if people are detected in the area while the auxiliary shutter is opened, an alarm must sound and the auxiliary shutter must close. If the shutter cannot be closed rapidly enough to limit possible personnel radiation exposure to an acceptable limit, this interlock must also interface to the accelerator system, inhibiting the proton beam. The interlock system will be monitored by the SNS Personnel Protection System. Access interlocks will conform to the SNS Personnel Protection System standards. For seismic safety requirements see 7.1.

Appendix:

Scattering geometries in commercial X-ray diffraction systems and the usefulness of an Eulerian cradle

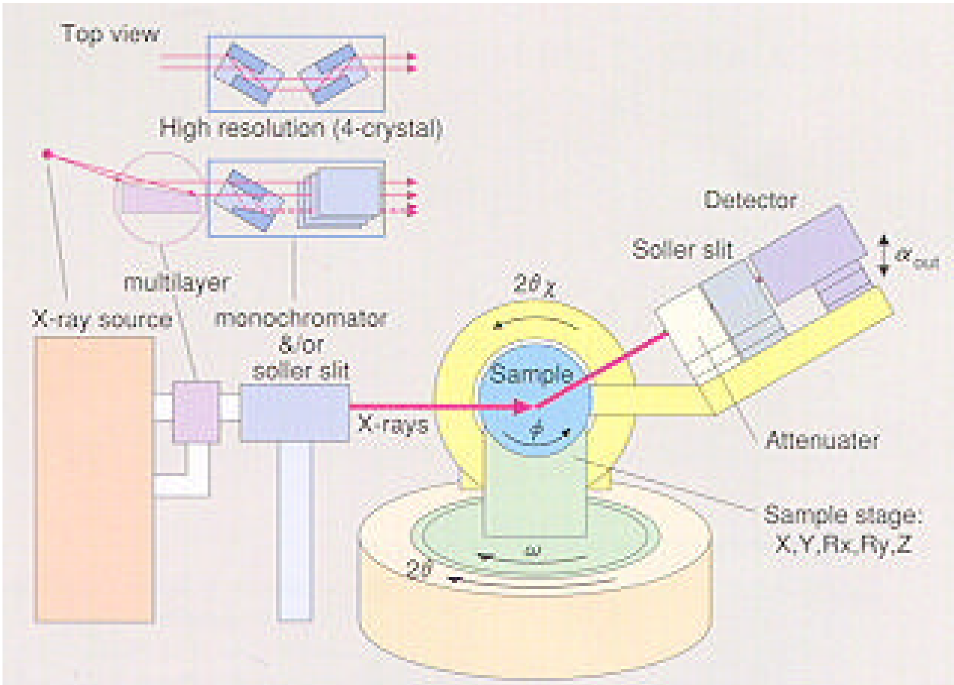
The companies BRUKER and PHILIPS use an Eulerian cradle as a key element in their X-ray diffractometer units. Similar to the Magnetism Reflectometer these systems use a vertical sample surface configuration for reflectometry experiments. However, for grazing incidence in-plane diffraction experiments they change to a horizontal configuration. They achieve the necessary 90 deg. turn of the sample by an Eulerian cradle that is mounted on the goniometer.

Fig. 22 shows the BRUKER setup: The sample can be moved from the vertical surface arrangement (for reflectometry) into a horizontal one for grazing-incidence diffraction experiments.

Fig. 22: X-ray diffractometer (BRUKER)

The RIGAKU company also uses a vertical sample surface geometry for reflectometry experiments. However, for grazing incidence diffraction experiments (scattering vector within the sample surface) they use an additional detector motion axis.

Fig. 23 shows the RIGAKU setup:



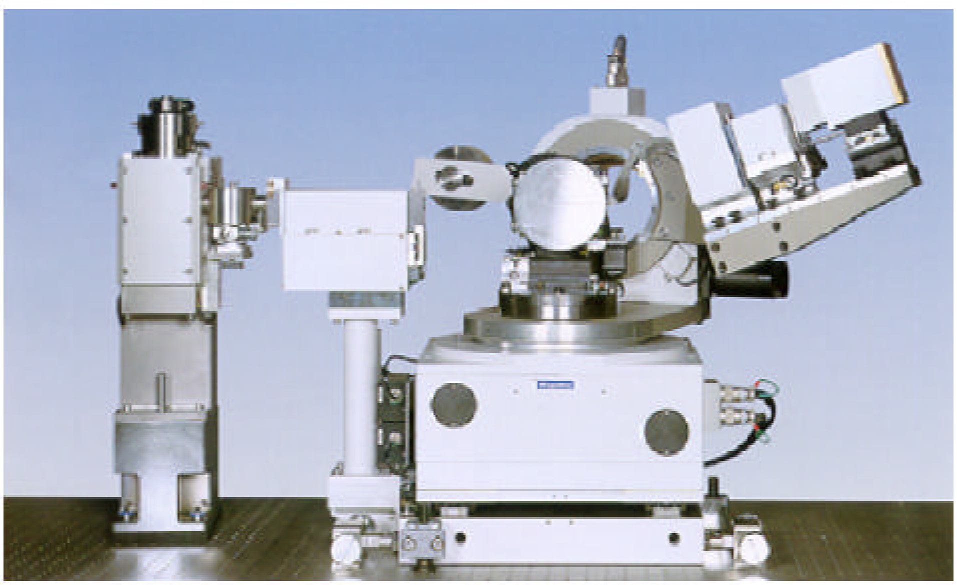


Fig. 23: X-ray diffractometer (RIGAKU),
top: schematic arrangement, bottom: the actual device

The adaptation of this arrangement for the Magnetism Reflectometer design would imply the drawback that the detector needs to be moved vertically, which is an engineering challenge. In extreme positions, i.e. at high Q-values, the heavy detector assembly (detector, optical elements and shielding) would need to be positioned vertically above the sample area.

As can be seen, for X-ray diffraction systems both possibilities operate successful. However, for the SNS Magnetism Reflectometer the Eulerian cradle solution seems to be much better suited since in this approach the additionally required 2θ movement of the detector (see Fig. 23) can be avoided. An additional benefit when employing an Eulerian cradle is that diffraction measurements in arbitrary lattice directions would be possible. Furthermore, no changes in the analyzer/detector system are required, when changing the sample orientation from vertical to horizontal.

One should note that Eulerian cradle systems with integrated sample stage (including heating and cooling capabilities) are commercially available. It needs to be determined if a magnet system of sufficient strength can be incorporated in an Eulerian cradle setup.

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