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# Optical Components for the Extended Q-Range Small Angle Diffractometer at the SNS

Jinkui Zhao

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# 1. Introduction

The Extended Q-Range Small Angle Scattering Instrument (EQ-SANS) [1] (Fig. 1) on the 60Hz SNS target is designed to have high intensity, high precision, and large Q-coverage. The machine is located on beam line No. 6, facing the downstream, upper, coupled hydrogen moderator. Its total length is variable between 15 and 18m or higher, depending on engineering optimization. This document describes the design choice of the optical system on the EQ-SANS.



Figure 1. Conceptual sketch of the EQ-SANS adapted from [1].

# 2. Design Choices

The Extended-Q SANS is designed to have a beam size of  $40x40 \text{ mm}^2$ . Thus, all the guide and benders on the Extended-Q SANS will have corresponding inner cross-sections to transport neutron beams of  $40x40 \text{ mm}^2$  in size. The guide system consists of three parts, a straight section within the target core vessel insert, a true curved bender within the beam shutter and the bulk shield and sections of straight guides following the bender (Fig 2). The supermirror coating of the guides and bender has a critical reflection of angle of 3.5m, namely 3.5 times the natural nickel (m=3.5, or 3.5 x 0.1°/Å). The exception is the convex side of the inner bender blades, which have m=2.

The initial straight guide section within the target core vessel insert is 39.37 inches (1.0 m) long. Preceding the guide is a section of 10.68-inch (271 mm) iron collimator with the opening cross-

section of 40x40 mm<sup>2</sup>. The core vessel insert is water-cooled and the guide is thermally coupled with the insert with helium at atmospheric pressure. The calculated energy deposition on beam line 6TD is found in attachment A1. Temperature calculation for the core vessel inserts on this beam line is ongoing. Calculated temperature from other beam lines with higher energy deposition does not indicate a risk to the core vessel guide under normal operational condition.

The multi-channel bender is separated in two parts. The first part is 72.76 inches  $(1.85 m) \log m$  and is located in the beam shutter. The second part is 47.60 inches  $(1.21m) \log m$  and is located in the bulk shield following the shutter. The bender is designed to be 'true-curved', i.e. it shall follow the perimeter of an arc. The radius of curvature of the bender arc is 2683 inches (68.1 m).

Following the bender, there is a straight guide section 94.99 inches (2.41m) long. A T0 chopper is foreseen for future upgrade immediately following the first disk chopper. The addition of a T0 chopper will change the total length of the straight guide.



Figure 2. Schematic of the optical system on the EQ-SANS.

## 2.1 Multi Channel Beam Bender

The multi channel beam bender is horizontally bent and is designed to avoid the direct line of sight of the neutron moderator from the sample position. Thus, bringing the shield material as close to the neutron beam as possible is essential for ensuring the bender to fulfill its designed

function. Especially critical is the guide glasses on the left and right sides of the bender. They have to be as thin as reasonable. The glasses on the top and bottom sides of the benders can be relatively thick to provide mechanical stability for the bender. The maximum distance between the supermirror coating of the side glasses and the bender enclosure (which acts at shielding material) is designed at 5 mm (The thinner the better). The maximum distance between the supermirror coating of the top and bottom glasses and the bender enclosure will be 10 mm.

The bender enclosure act as shielding and provides the needed vacuum for the bender. This will apply to venders that have an interest of providing the guide and enclosure as a complete system.

The number of blades in the bender is chosen at 7, providing 8 channels. Fewer channels (6 or 7) are acceptable, depending on the manufacturing difficulties of the bender. The blades should be 0.3mm or thinner. The final thickness of the blades shall be determined by consultation between the SNS and the vendors. Thicker blades may be acceptable, but it will influence the decision on the number of blades needed, as thicker blades will take more spaces and few blades may be needed in such cases.

The supermirror coating of the bender top and bottom walls, the side walls and blade inserts on the concave side, shall be m=3.5 with 65% reflectivity or better. Alternative options with m=3 and 80% reflectivity with be considered as well. The coating on the convex side of the sidewalls and blade inserts shall be m=2, with 90% reflectivity or better.

The bender shall be curved and following an arc with the radius of curvature of 2683 inches (68.1 m). It is consisted of two segments, one 72.76 inches (1.85 m) long and is located in the beam shutter and one 47.60 inches (1.21m) long and is located in the bulk shield. Each of the two segments can be break in two smaller sections to facilitate manufacturing. The gaps between these subsections should be minimized. The exact number of sections will be determined in consultation between the SNS and the venders.

# 2.2 Guides

There are two segments of the straight guides on the Extend-Q SANS, one is upstream from the bender (toward the target and moderator) and one is downstream from the bender. The guide upstream from the bender shall be 39.37 inches (1.0 m) in length. The guides downstream from the moderator shall be consisted of two subsections.

The requirement on glass thickness is the same as that for the bender sidewalls. The maximum distance between the supermirror coating of the left and right side glasses and the guide enclosure should be 5 mm. The maximum distance between the supermirror coating of the top and bottom glasses and the guide enclosure should be 10 mm. The final thickness value will be the same as for the bender and will be determined in consultation between the SNS and the vendors.

The supermirror coating on the guides is designed to be the same as the top and bottom walls of the bender, namely m=3.5 with 65% reflectivity or better. An alternative option is m=3 and 80% reflectivity.

# 3. Performance calculations and optimizations

The optical system is optimized both analytically and by using Monte Carlo simulations. Analytical optimizations were mostly focused on the beam cross section and the bender bending curvature, whereas Monte Carlo Simulations were used to verify various design options. Unless otherwise noticed, all Monte Carlo simulations here use the program IB (Zhao/SNS) and the moderator source file source\_sns89\_td\_14.dat provided by Eric Iverson of SNS, scaled 2MW. The simulation condition is the same as that for the conceptual design document [1].

# 3.1 Curvature and length of the beam bender

The choice of bender length and curvature is guided fore mostly by the need of blocking the direct line-of-sight of the moderator as early as the neutronic performance of the optical system allows. Avoiding the direct line of sight further upstream enables better background shielding for experiments with weak scattering signals. The length of the bender is further limited by two constraints. First, it is undesirable to have the bender in the core vessel, as operational uncertainties may cause temperature to rise in that region and thus damage the bender. Therefore the bender will have to start from within the primary beam shutter, which is ~ 2.3 m away from the moderator. Second, because the first bandwidth chopper is best located right at the bulk shield liner (~5.5m) and because a T0 chopper after the first disk chopper may be necessary in the future, it is undesirable to have the beam bender extending beyond the choppers, especially the T0 chopper. A bending radius of R~65m and arc length of L~3m is found to suit the bender needs. Engineering optimization further refined these parameters to R=68.1m and L=3.06m.

The performance of benders with different bending radii are also simulated and shown below.



Figure 3. Transmission comparison between benders with bending radii of 50m and 65m[1]. For smaller bending radii, more bender channels are needed to obtain comparable transmission performance.



Figure 4. Relative bender transmission to a straight guide for larger bender radii. For these large bending radii, longer benders than the used 3m will be needed, which are less desirable for engineering design reasons (see text).



Figure 5. Relative bender transmission to a straight guide for a bender with a 150m bending radius with different number of channels. R=150m is not chosen because it is less desirable for engineering design reasons (see text).

## 3.2 Number of bender channels

In the conceptual design document [1], the optimal number of bender channels is found at 10. However, manufacturing difficulties may put further constraint on channel number, either because of the finite thickness of the blade inserts, or because of the manufacturing costs. Fewer channels down to 6 will be acceptable. With even fewer channels, the high-Q performance of the instrument will suffer increasingly because of the low transmission rate of short wavelength neutrons.



Figure 6. Left: Relative transmissions of 6, 10, and 14 channel benders when compared to a straight guide. Right: Transmission ratio between 6, 14 channel benders and a 10 channel bender.

## 3.3 Guide coatings

#### **Coating on Straight guides**

Because the EQ-SANS is designed to have a shortest sample to detector distance of 1m, divergent neutrons with 1m collimation can be used. Therefore, not only the bender, but also the straight guides should have a supper mirror coating with high critical reflection angle. The following graph shows the performance increase of supermirror coated guides after the bender when compared to nature nickel guides.



Figure 7. Effect of different the straight guide coatings (between 5-13m) on the neutron flux at the sample position (14m) with a 1m collimation length [1].

#### **Coating of the Bender**

The concave side of the bender side wall and inner blades bears the most burdens in bending the thermal and cold neutrons and should have the highest coating that is reasonable. However, on the convex side, the coating requirement can be relaxed. These figures show the absolute transmission of benders with convex side coatings of 2x Ni  $\theta$ c and 90% reflectivity comparing to uniform, higher indexed coatings.



Figure 8. Absolute bender transmission (with 1° source divergence). (a)  $3.5 \times \text{Ni} \ \theta \text{c}$ , 70% reflectivity coatings (purple line) and (b) same coatings as in (a) except that  $2 \times \text{Ni} \ \theta \text{c}$ , 90% reflectivity coatings were used for the convex side of the bender wall and inner inserts. The reflectivity of the supermirrors at the natural Ni critical angle is set to 98%.



Figure 9. Absolute bender transmission (with 1° source divergence). (a) 3 x Ni  $\theta$ c, 80% reflectivity coatings (purple line) and (b) same coatings as in (a) except that 2 x Ni  $\theta$ c, 90% reflectivity coatings were used for the convex side of the bender wall and inner inserts. The reflectivity of the supermirrors at the natural Ni critical angle is set at 98%.

### 3.4 Vertical guide and bender height

In principle, the height of beam cross section defined by the guide system on the EQ-SANS can be larger than its width. Since the beam is bent in the horizontal direction, higher beam cross sections will not impact the line-of-sight of the moderator. However, simulations show that higher guides and benders do not bring the anticipated higher flux at the sample position under normal operational condition (square or circular samples).



Figure 10. Flux at the sample position with 4m collimation vs. Guide-height. The sample size is kept at 2cmx2cm.

### 3.5 Gaps in the guide system

Gaps in the guide system and losses of a section of the guide will have the most impact on experiments with the shortest collimation lengths. Possible large gaps are the addition of a T0 chopper for reducing the fast neutron background. Possible guide loss is the 1m straight guide in the core vessel insert. In order to reduce the fast neutron background as much as possible, an

inversely tapered collimator at the core vessel insert in place of the straight guide is not desired. The lost of the core vessel guide is neutronically equivalent to having a collimator in place. The simulations show that the core vessel guide will increase the flux at the sample position for short collimation lengths, but the lost of it will not drastically impact the performance of the instrument.



Figure 11. Effect of a 50cm T0-Gap in the guide system at 5.5m on the flux of neutrons with a maximal 1° divergence at the sample position [1]



Figure 12. Moderator to sample simulation with and without the core-vessel guides. Left: relative fluxes at the 2cm x 2cm sample with a 1m collimation length (from the end of the guide system to the sample). Right: relative guide gain. The simulation conditions are as the following: (1) The moderator source generates neutrons between 1-15Å with a max divergence of 1°. (2) A slit is located at 1m from the moderator. This is the place where the core-vessel starts. (3a) For simulations with the core-vessel guide: a slit is placed at 1.27m from the moderator and a 1m guide after that. (3b) For simulations without the core-vessel guide: a slit is placed at 2.27m. (4) A curved bender 3.06m long with the radius of curvature of 68m. (5) A straight guide is placed between 5.35 - 13m from the moderator. (6) A 2cmx2cm detector is placed at the sample position of 14m from the moderator. All slits, guides and benders have the same cross-section of 4cmx4cm. The super-mirror coating for the guides and benders is 3.5xNi- c, except the convex on the side of the bender, which is 2x. These geometrical parameters reflect the actual engineering design and differ slightly from those of the conceptual design

# 4. Alternatives to the true curved bender

## 4.1 The combination of straight guides with a T0 chopper.

This is one of the early choices we have to make on this instrument. The bender system was chosen basically because of the uncertainty in fast neutron backgrounds and the ability of a T0 chopper to stop the fast neutrons. Neutronic performance of a straight guide with a T0 chopper is compared with the designed chopper here [1].



Figure 13. Neutronic performance comparison between the designed beam bender and an alternative of replacing the bender with a straight guide and adding a T0 chopper to block the fast neutrons. The calculated flux is at the sample position with 1m collimation length. The straight guide option clearly wins for shorter wavelength neutrons. For neutrons >5 Å, the bender wins under ideal condition (the thickness of the bender blades, for example, is not factored in for these simulations.). This is because the 50cm T0-gap in the straight-guide option causes neutron losses.

### 4.1 Segmented Bender

#### Ignoring the divergence degradation

Polytonally approximation of a true curved bender with short segments of straight, multi-channel guides offers the advantage that it has a sharp cutoff for fast neutrons. It may very well be easier to manufacture than the true curved one as well. On instruments that use divergent neutrons, segmented benders offer even a slightly higher transmission in certain wavelength range (see graph below).



Figure 14. Absolute transmission (left) and transmission ratio of the guide system with segmented bender comparing to the designed, curved bender. All benders are 3m-long. The source divergence of 1° is used in the simulation. All neutrons exiting the bender are counted.

#### Preserving the neutron divergence

When those neutrons that exit the bender with larger divergence than fed-in divergence to the bender system are discounted, the curved bender outperforms segmented ones in most cases. Since collimation and divergence is a very important factor for the performance of a SANS instrument, a true curved bender is preferred to a segmented one [refer also to reference 2]. Below are comparisons between segmented and curved benders under different divergent constraints.



Figure 15. Relative transmission of segmented benders to the designed curved bender. For the solid lines, all neutrons exist the bender are counted. For the dotted lines, only exiting neutrons with divergences less than or equal to the input divergence are counted. The maximum neutron divergence generated at the source is 0.1°.



Figure 16. Relative transmission of segmented benders to the designed curved bender. For the solid lines, all neutrons exist the bender are counted. For the dotted lines, only exiting neutrons with divergences less than or equal to the input divergence are counted. The maximum neutron divergence generated at the source is 0.2°.



Figure 17. Relative transmission of segmented benders to the designed curved bender. For the solid lines, all neutrons exist the bender are counted. For the dotted lines, only exiting neutrons with divergences less than or equal to the input divergence are counted. The maximum neutron divergence generated at the source is 0.5°.



Figure 18. Relative transmission of segmented benders to the designed curved bender. For the solid lines, all neutrons exist the bender are counted. For the dotted lines, only exiting neutrons with divergences less than or equal to the input divergence are counted. The maximum neutron divergence generated at the source is 1°.

# References

- Conceptual Design and Performance Analysis of the Extended Q-range, High Intensity, High Precision Small Angle Diffractometer for SNS, May 2000, Jinkui Zhao, SNS report No. IS-1.1.8.2-6036-RE-A-00
- 2. Monte Carlo Simulations on Spectrometers for SNS, P Yuan and J Zhao, SNS report No. 107000000-TR0004-R00

### Attachments

A.1. Energy deposition on beam line 6TD calculated by Brian Murphy (SNS Doc ???????)



Fig A1. (Supplied by Brian Murphy) The plot shows heating in the various materials of the beam tube as a function of distance from the moderator face. This beam tube was in position #6 meaning that it is one of the three that face the top, downstream (coupled) moderator unit. This beam tube contains a glass neutron guide on the inside of which is a thin nickel layer. There is a narrow gap between the glass guide and the surrounding stainless steel body of the beam tube. A cadmium layer, within this gap, surrounds the guide and acts as a neutron shield. The upstream edge of the glass guide is located 28 cm downstream from the upstream edge of the insert (beam tube). Upstream of the glass guide section the beam tube contains a stainless steel collimator inside the main stainless steel body of the unit. In the plot these two sections are identified as the collimator and guide sections respectively.

The opening is not in the center of the beam tube. It is offset such that it points towards the section of the moderator face producing the maximum neutron flux. This section is towards the upstream edge of the moderator and it is also towards the bottom of the moderator (i.e., nearer the target).