# Neutron Optics Optimization for the SNS EQ-SANS Diffractometer

**Jinkui Zhao**

Neutron Scattering Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA

**Abstract**

The extended *Q*-range small angle neutron scattering (EQ-SANS) diffractometer at the Spallation Neutron Source has recently been completed. Initial commissioning has shown that it has achieved its high intensity, low background, and wide dynamic range design goals. One of the key components that enable these performances is its neutron optics, which are extensively optimized using analytical and Monte Carlo methods. The EQ-SANS optics consist of a curved multichannel beam bender and sections of straight neutron guides on both ends of the bender. The bender and the guide are made of float glass coated with supermirror multilayers. The function of the optics is to ensure low instrument background by avoiding the direct line of sight of the neutron moderator at downstream locations, while transporting thermal and cold neutrons to the sample with maximum efficiency. In this work, the optimization of the EQ-SANS optics is presented.

**Keywords** Neutron optics, multichannel beam bender, SANS, Spallation Neutron Source, Monte Carlo Simulations.

## 1. Introduction

One of the major design challenges of a high performance small angle neutron scattering (SANS) diffractometer on a spallation neutron source is how to maximize neutron flux on sample and minimize instrument background in the same time. The difficulty is especially great when the repetition rate of the source is high. When the rep rate is high, the length of a SANS instrument has to be short in order for the instrument to have a wide wavelength band, which is needed to increase the total neutron flux on sample. On the other hand, a short instrument complicates background shielding. Spallation neutron sources produce large amounts of fast neutrons at time zero, namely at the time when an accelerated proton pulse strikes the target and a neutron pulse is generated (prompt pulse). These fast neutrons are a main source of instrument background. Due to their very high energy, shielding against them is extremely difficult. One novel approach in new generations of SANS diffractometers is to use multichannel beam benders to change the direction of thermal and cold neutrons and to get away from the direct line of sight from the neutron moderator (i.e. neutron source). Many meters of shielding materials, commonly steel and concrete, are then stacked after the last direct-line-of-sight point to block these fast neutrons. The flight direction of fast neutrons cannot be bent by the beam bender. The newly commissioned EQ-SANS diffractometer [1] at the Spallation Neutron Source (SNS) is one such instrument. Its optics use a combination of a multichannel beam bender and straight neutron guides. The last direct line of sight from the moderator on the instrument is ~6m upstream from the sample, allowing ample amount of shielding spaces. The optics transport thermal and cold neutrons with very high efficiency, making it possible for the EQ-SANS instrument to achieve its high performance.

## 2. Design Summary

Figure 1 shows the schematic presentation of the EQ-SANS beam optics. Figure 2 shows photos of selected optical components. The optics has a beam cross section of 40×40mm$^2$. It starts in the core vessel insert of the SNS target station with a 270mm long steel collimator, followed by a 1m long section of straight neutron guide. Located in the primary beam shutter and the bulk shield insert of the SNS target station is a 3.3m long, 6 channel, curved beam bender. The bender follows an arc with the radius of 95m. Beyond the bulk shield insert are ~ 4m of straight neutron guides and two additional meters of removable guides (the second meter is to be installed). The optics is manufactured by SwissNeutronics Inc [2] with the following parameters: all of the benders and guides are coated with supermirror multilayers with the critical reflection angle of $3.5\times\theta_c$, except the convex sides of the bender channels, which have $2\theta_c$ supermirrors ($\theta_c$ is the critical reflection angle of natural nickel); the reflectivity is ≥70% for the $3.5\theta_c$ coatings and ≥90% for the $2\theta_c$ coatings.

## 3. Design Optimization

The EQ-SANS diffractometer is intended to be a workhorse for the SNS. It is a short instrument with 14m of primary flight path [1]. Because the instrument has pinhole geometry and requires collimation space upstream from the sample, the fixed portion of its optics is designed to terminate at 10m from the moderator. In the current work, the optimization process for the EQ-SANS optics is constraint under this condition. In addition, the width of the beam (40mm) is considered to be optimal for the EQ-SANS, since its typical scattering samples are 20mm or less in size. Nonetheless, options for higher beams are explored. The neutron beam is curved in the horizontal direction. So a higher beam does not affect its bending. Other parameters that are optimized include the number of bender channels, the radius of bender curvature, and the supermirror multilayer coatings etc. The main optimization goal is to maximize the transport of thermal and cold neutrons and to avoid the moderator direct line-of-sight as upstream from the sample position as possible.

### 3.1 Monte Carlo Simulation Conditions

The parameters of the EQ-SANS optics as described in section 2 and figure 1 (without the last two pieces of removable straight guides) are used as the baseline design for the simulations and performance comparisons. Unless otherwise stated, a $40\times40mm^2$ collimation slit and a $20\times20mm^2$ sample slit are located at 10m and at 14m from the moderator, respectively. The detector is located immediately after the sample slit. The reflectivity for the supermirror coatings are set to 98% at $\theta_c$, 90% at $2\times\theta_c$ for the convex side of the bender walls, and 70% at $3.5\times\theta_c$ for the rest of the optics. The moderator spectra are obtained from reference [3]. Neutrons are generated at the source with ±1° divergence, which is sufficient to fully illuminate the optical system with the 4m collimation setting for the simulations. The simulations were performed using the Monte Carlo program IB [4]. The statistics presented here corresponds to $10^{11}$ neutrons generated at the neutron source and on the order of $10^8$ neutrons detected at the sample location.

### 3.2 Bender versus Straight Guide

Alternative to using a multichannel beam bender is to use a straight neutron guide in combination with a T0 chopper. A T0 chopper is a large piece of dense material, such as steel, that rotates into the neutron beam at time zero to block the fast neutrons and gamma rays from the prompt neutron pulse. Figure 3 shows the simulated relative transmission of the EQ-SANS optics as compared to a straight guide alternative. The transmission is defined as the ratio of neutron counts at the sample location versus the number of neutrons that enter the optics. The relative transmission is obtained from the transmission of EQ-SANS optics divided by that of the straight guide alternative. For cold neutrons with wavelength $\lambda > 5$Å, the EQ-SANS optics and the alternative straight guide transport neutrons with about the efficiency. Either of these two options will deliver about a 9× flux gain when compared to no optics in the beam. The EQ-SANS optics thus offer the instrument an excellent cold neutron performance. For shorter wavelength neutrons, the straight guide option has a clear advantage. However, with the straight guide, the operation and maintenance of the required T0 chopper is very burdensome. Even with a lower optical transmission for short wavelength neutrons, the flux on sample at these wavelengths on the EQ-SANS is still sufficiently high (figure 3) to allow the instrument to effectively extend its neutron momentum transfer ($Q$) coverage to larger $Q$-values.

### 3.3 First Section of Guide

Since the EQ-SANS diffractometer is a short instrument, its optics need to be close to the source in order for the instrument to avoid the moderator direct line of sight early on. Energy deposition calculation and thermal analysis have predicted that, after a short piece of collimator (figure 1), neutron optics can indeed start within the core vessel insert of the

SNS target station without significant risks of being damaged by the neutron source [5,6]. Nonetheless, placing a multichannel beam bender inside the core vessel still carries some operational risks, since a damaged beam bender may render the instrument unusable. Therefore, the EQ-SANS optics starts with a 1m long straight guide (figure 1). This guide section increases the flux on sample by as much as 20% when compared with the case where the guide is replaced with a collimator (figure 4). Opening up the collimator to allow the multichannel beam bender that follows (figure 1) to have a full view of the neutron moderator can achieve the same flux gain, but at the expense of shifting the direct line of sight of the moderator further downstream, creating more burden for background shielding.

### 3.4 Bender Length, Radius, and Number of Channels

The length of the multichannel beam bender (3.3m) is largely constraint by the physical dimensions of the primary beam shutter and the bulk shield insert of the SNS target station. On the downstream end of the bender, the first bandwidth chopper is located in the target station's chopper cave on the perimeter of the target monolith (figure 1, [1]). Extending the bender beyond this first bandwidth chopper is possible. However, spanning multichannel benders across a bandwidth chopper creates concerns for accurate alignment. In addition, benefit of a longer bender can also be obtained from optimizing other bender parameters, such as the bender curvature and the number of channels.

The radius of curvature and the number of channels first and foremost affect the bender transmission for short wavelength neutrons. With a larger radius (R=150m, figure 5) or more channels (10 channels, figure 5), for example, the bender performance increases for <2Å neutrons. However, each of these options has a disadvantage. A larger bender radius pushes the last direct line of sight of the moderator further downstream. More channels mean that more materials in the beam to attenuate the flux, especially for cold neutrons. The thinnest non-borated glass that was available as bender inserts for the EQ-SANS optics is ~0.55mm thick [1].

### 3.5 Supermirror Coating

Supermirror multilayers with large critical reflection angles and high reflectivity are essential for the performance of the EQ-SANS optics. This is evident from figure 6, which shows the relative transmission of a Ni coated EQ-SANS optics ($1\times\theta_c$). Within the divergence limit set by the 4m collimation (see section 3.1), the Ni coated optics will transport neutrons only effectively for > 7Å neutrons. The effect of the mirror reflectivity is also demonstrated in figure 6. For the Ni simulation, the reflectivity at $\theta_c$ is assumed to be 100%, which results in a better transmission for colder neutrons than the EQ-SANS optics. The latter uses a reflectivity of 98% at $\theta_c$ for the simulation (see section 3.1).

The curved nature of the EQ-SANS bender means that the multilayer coatings on the convex sides of the bender walls can have a smaller critical angle than the concave side. In fact, with its $2\theta_c$ coating on the convex sides of the channels, the EQ-SANS optics has a slightly better simulated transmission for <2.5Å neutrons than if the bender were coated with $3.5\theta_c$ multilayers on all sides (figure 6). Similar to the above discussion on Ni coated guides, the difference arises from the fact that the $2\theta_c$ multilayers have a higher reflectivity than the $3.5\theta_c$ coatings at the reflection angle of $2\times\theta_c$. Such difference may not be significant for the actual bender due to variations in multilayer manufacturing. In any event, replacing the convex side of the EQ-SANS bender with the much less expensive $2\theta_c$ multilayers will not degrade its performance.

### 3.6 Guide Height

Because the EQ-SANS beam bender curves in the horizontal direction only, it is tempting to look into options of having a higher beam cross section. A higher beam will not affect the avoidance of the direct line of sight of the neutron moderator, but will bring more neutrons toward the sample area. However, since the EQ-SANS has pinhole geometry, the collimation and sample slits need to be either square or circular for most experiments. Under such constraints, higher beam cross section for the optics will not benefit the flux on sample (figure 7).

## 4. Performance

At the exit of the multichannel bender, the neutron flux is fairly evenly distributed for cold neutrons (data not shown). This is not the case at shorter wavelength due to garland reflections (figure 8). However, after the additional three sections of straight neutron guides (figure 1), this unevenness becomes insignificant (figure 8).

For SANS instruments, the most important performance criterion for the optics is to maximize the flux at the sample location and to minimize the instrument backgrounds due to fast neutrons from the prompt pulse. Figure 9 shows the simulated and measured fluxes on the EQ-SANS instrument constructed with the presented optics. The comparisons are performed for two configurations: One is for the flux at the end of the neutron guides with no collimation. The other is at the sample location, which is 4 m away from the optics. It is apparent that the EQ-SANS optics perform largely as expected. We note that the measured fluxes are ~25% lower than simulated ones. There are two apparent factors that can contribute to this discrepancy. The as-built EQ-SANS optics have 10 mm thick of vacuum window materials along the beamline. There are additional 4 mm of window materials from the beam monitor which is located at the end of the neutron guides [1]. These 14 mm thick materials are made of aluminum alloys, which can attenuate the neutron beam by ~10% for 5 Å neutrons and ~ 20% for 20 Å ones. Additionally, the as-built optics will not have the perfect manufacturing, installation, and alignment accuracies as were assumed in the simulations, further decreasing the flux at the sample. These imperfections are also apparent in the spectra for short wavelength neutrons, where the measured flux drops off faster than the simulations as the neutron wavelength decreases. Because the neutron total reflection angle decreases with wavelength, these imperfections will have more impact on neutrons with shorter wavelength.

## Acknowledgements

During the course of its design, the EQ-SANS instrument and its optics have gone through numerous reviews. The author is grateful to all those who have offered useful discussions and suggestions.

This manuscript has been authored by UT-Battelle, LLC, under Contract No. DE-AC05-00OR22725 with the U.S. Department of Energy. The United States Government retains,

**References**

[1] J.K. Zhao, C. Y. Gao, and D. Liu "The Extended Q-Range Small Angle Neutron Scattering Diffractometer at the SNS" *J. Appl. Cryst.* 43 (2010) 1068-1077.

[2] *www.swissneutronics.ch.*

[3] E. B. Iverson, P. D. Ferguson, F. X. Gallmeier, and I. I. Popova,"*Neutronics calculations for scattering instrument design: SCT configuration*", SNS Document: SNS-110040300-DA0001-R00, Oak Ridge, TN, USA, (2002).

[4] J.K. Zhao "*IB: a Monte Carlo Simulation Tool for Neutron Scattering Instrument Design under Parallel Virtual Machine*". Submitted to NIM-A (2011).

[5] B. D. Murphy "*Extended Energy-Deposition and Damage Calculations in Core-Vessel Inserts at the Spallation Neutron Source*" SNS Document: SNS-107030600-DA0001-R01, Oak Ridge, TN, USA, April (2003).

[6] K. W. Childs "*Thermal Analysis of the 06td SANS Diffractometer Core Vessel Insert and Guide*" SNS Document: SNS-107080600-DA0005-R00, Oak Ridge, TN, USA, July (2003).

**Figure Captions**

Figure 1: Schematics of the optics system for the EQ-SANS instrument at the SNS. The gaps between the straight neutron guides sections outside the SNS target monolith are reserved for bandwidth choppers. The last two sections of the straight neutron guides are removable, and the very last section is to be installed.

Figure 2: Photographs of the EQ-SANS core vessel insert guide (left) and a section of the multichannel beam bender (right) in their respective steel casings.

Figure 3: Relative transmission of the EQ-SANS optics as compared to a straight guide (left axis), and the simulated flux on sample with the EQ-SANS optics (right axis). For the straight guide simulation, a 500mm gap is introduced in the optics to simulate the effect of a T0 chopper. The straight guide has the same $3.5\times\theta_c$ supermirror coatings.

Figure 4. Relative flux gain by the first meter of guide in the SNS core vessel, as compared to the same EQ-SANS optics with the core vessel guide removed.

Figure 5. Relative neutron transmissions of four alternative bender configurations with either different radius of curvature (symbols), or number of channels (lines), as compared to the EQ-SANS optics.

Figure 6. Relative transmission of alternative optical coatings as compared to the EQ-SANS optics. The dashed line is the transmission of Ni coated EQ-SANS optics ($1\times\theta_c$)

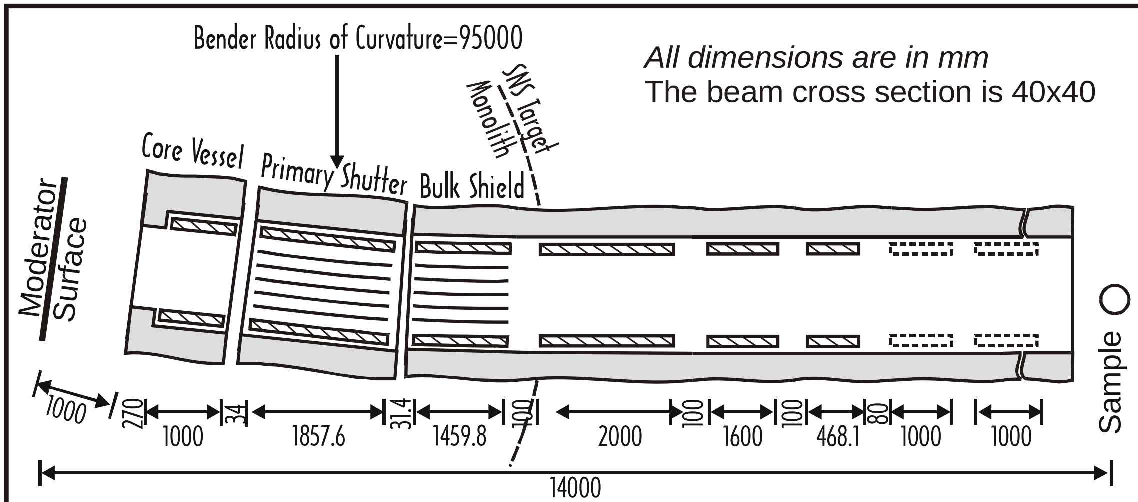
versus that of the actual optics. The solid line is when the convex side of the bender is coated with $3.5\times\theta_c$ supermirrors as well (see text for discussion).

Figure 7. Integrated flux between the wavelength of 2 and 10Å for different beam heights. The width of the optics is held at 40 mm. The $40\times40\text{mm}^2$ collimation slit and the $20\times20\text{mm}^2$ sample slit remain in place for all simulations. The flux drops at larger guide heights because when it reaches the height of the SNS moderator (120mm, [3]).

Figure 8. Upper: Simulated flux distribution across the neutron beam for 2Å neutrons at end of the multichannel beam bender. The garland-reflection is evident from the fact that neutrons are concentrated towards the outer walls of each channel. Lower: At the end of the straight neutron guides 10m from the moderator (figure 1). The simulation was performed with ±5° of source divergence, which is enough to over saturate the optics.

Figure 9. Simulated and measured fluxes on the EQ-SANS diffractometer, scaled to 1MW source power of the SNS target station. The red circles are measured flux at the sample position with a 4m collimation length. The measurement was taken by placing various sized pinholes at the sample location and using the EQ-SANS detector with corrections for wavelength dependent detection efficiency (92% at 1.8Å [1]) applied. The blue crosses are measured flux at the end of the optics with 0m of collimations. The data were collected using the beam monitor at the end of the optics, which is a low pressure gas detector with a calibrated absorption coefficient of $9\times10^{-5}\ \text{cm}^{-1}$.

Fig 1.

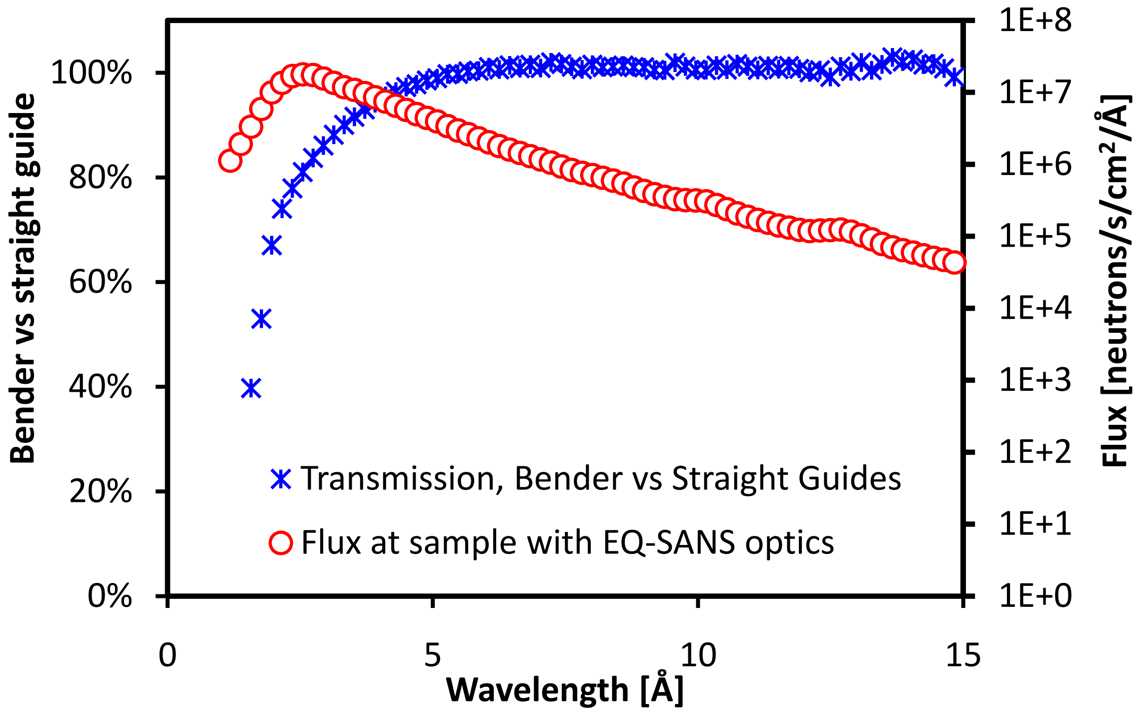



Hatched blocks : Glass wall for fixed guide & bender
Dashed blocks : Glass wall for removable guide
Shaded blocks : Steel shielding and vacuum boundary.

<u>Glass thickness</u>
(all elements use non-borated float glass):
Straight guides : CVI 5, others 3.
Bender top and bottom walls : 5; side walls: 1; inserts: 0.55.

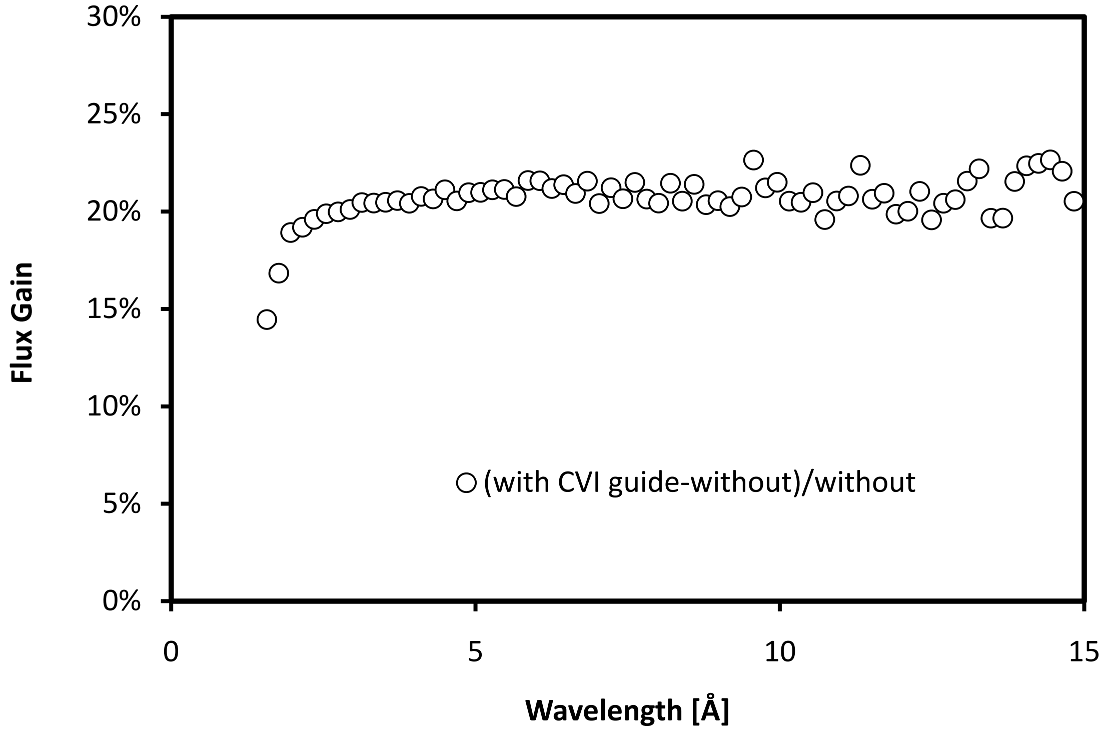
Fig 2.

Fig 3.



Bender vs straight guide
100%
80%
60%
40%
20%
0%
0
5
10
15
Wavelength [Å]
1E+8
1E+7
1E+6
1E+5
1E+4
1E+3
1E+2
1E+1
1E+0
Flux [neutrons/s/cm²/Å]
Transmission, Bender vs Straight Guides
Flux at sample with EQ-SANS optics

Fig 4.



30%
25%
20%
15%
10%
5%
0%
Flux Gain
(with CVI guide-without)/without
0
5
10
15
Wavelength [Å]

Fig 5

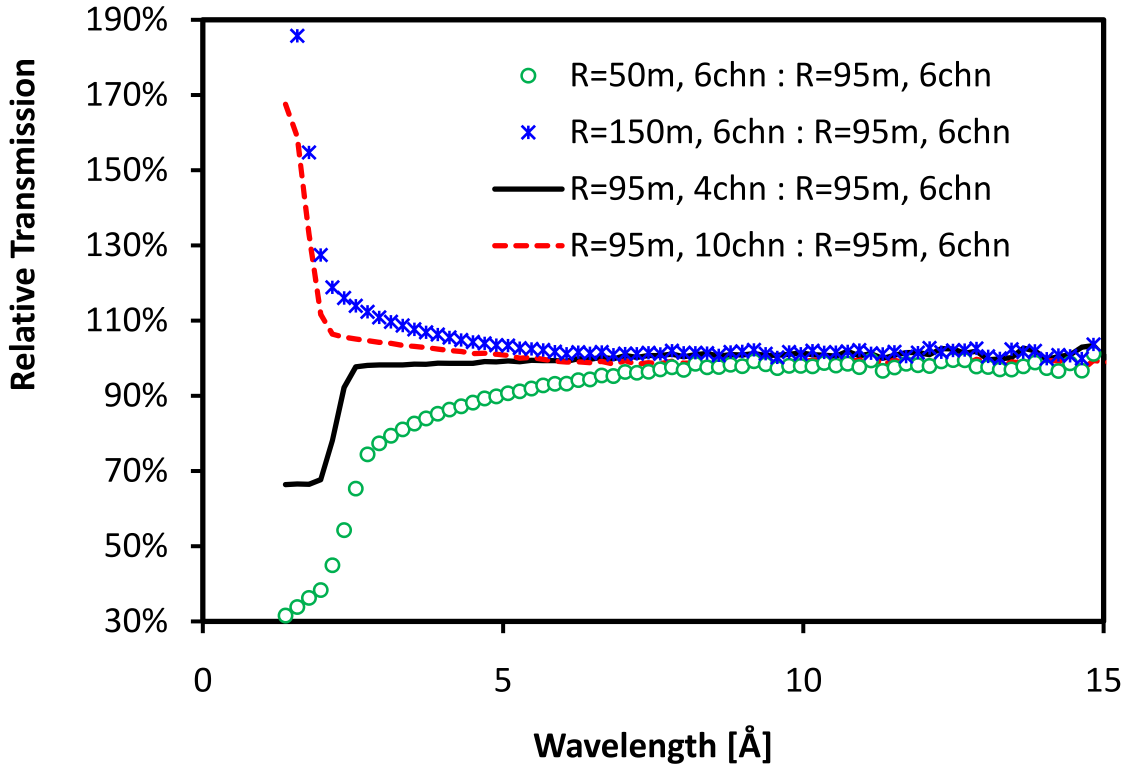

190%
170%
150%
130%
110%
90%
70%
50%
30%
0
5
10
15
Relative Transmission
Wavelength [Å]
R=50m, 6chn : R=95m, 6chn
R=150m, 6chn : R=95m, 6chn
R=95m, 4chn : R=95m, 6chn
R=95m, 10chn : R=95m, 6chn

Fig 6

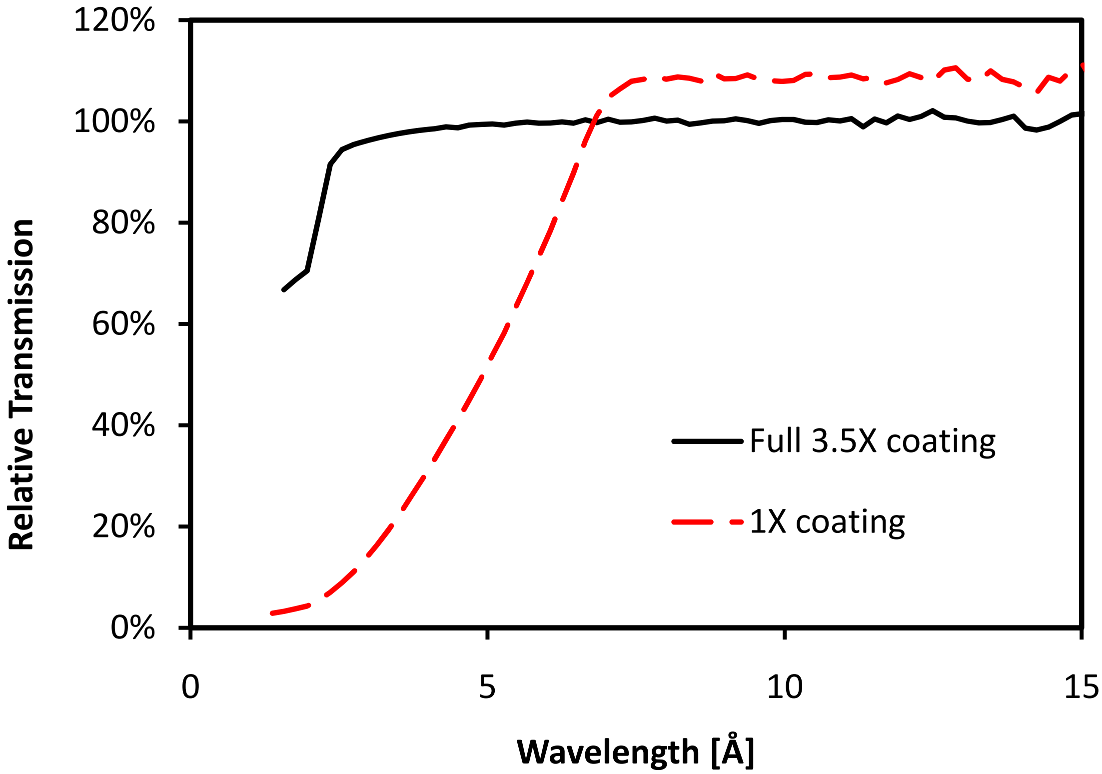

120%
100%
80%
60%
40%
20%
0%
Relative Transmission
0
5
10
15
Wavelength [Å]
Full 3.5X coating
1X coating

Fig 7

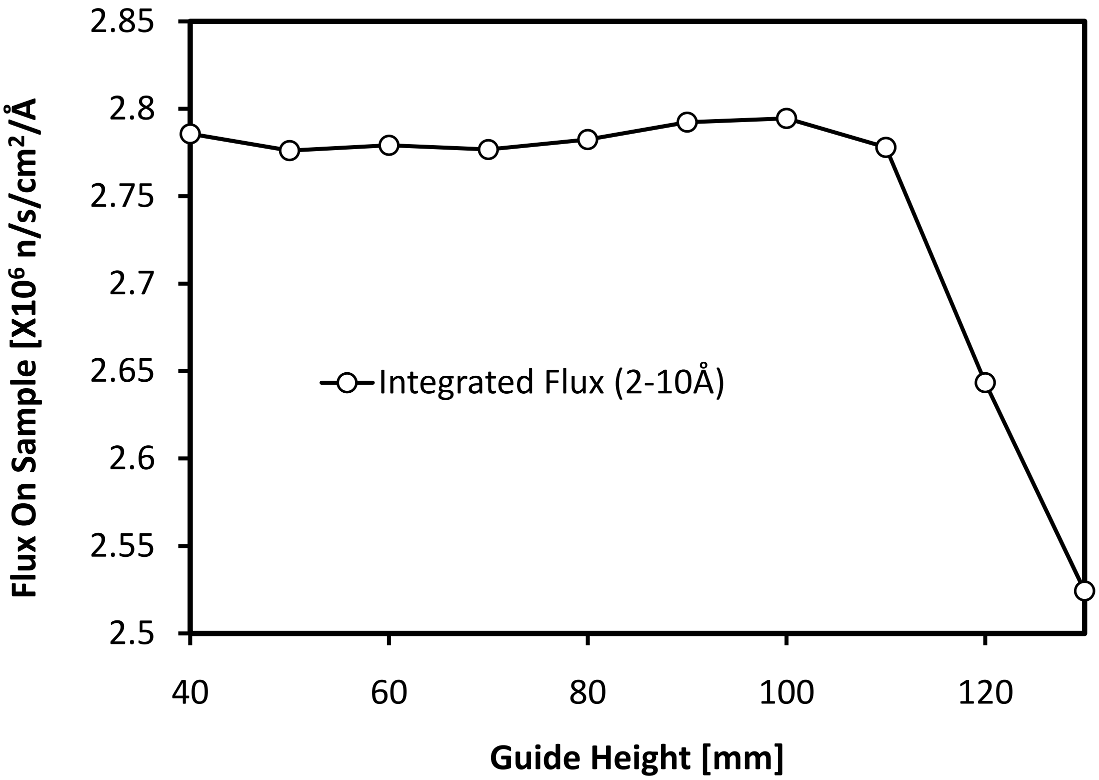
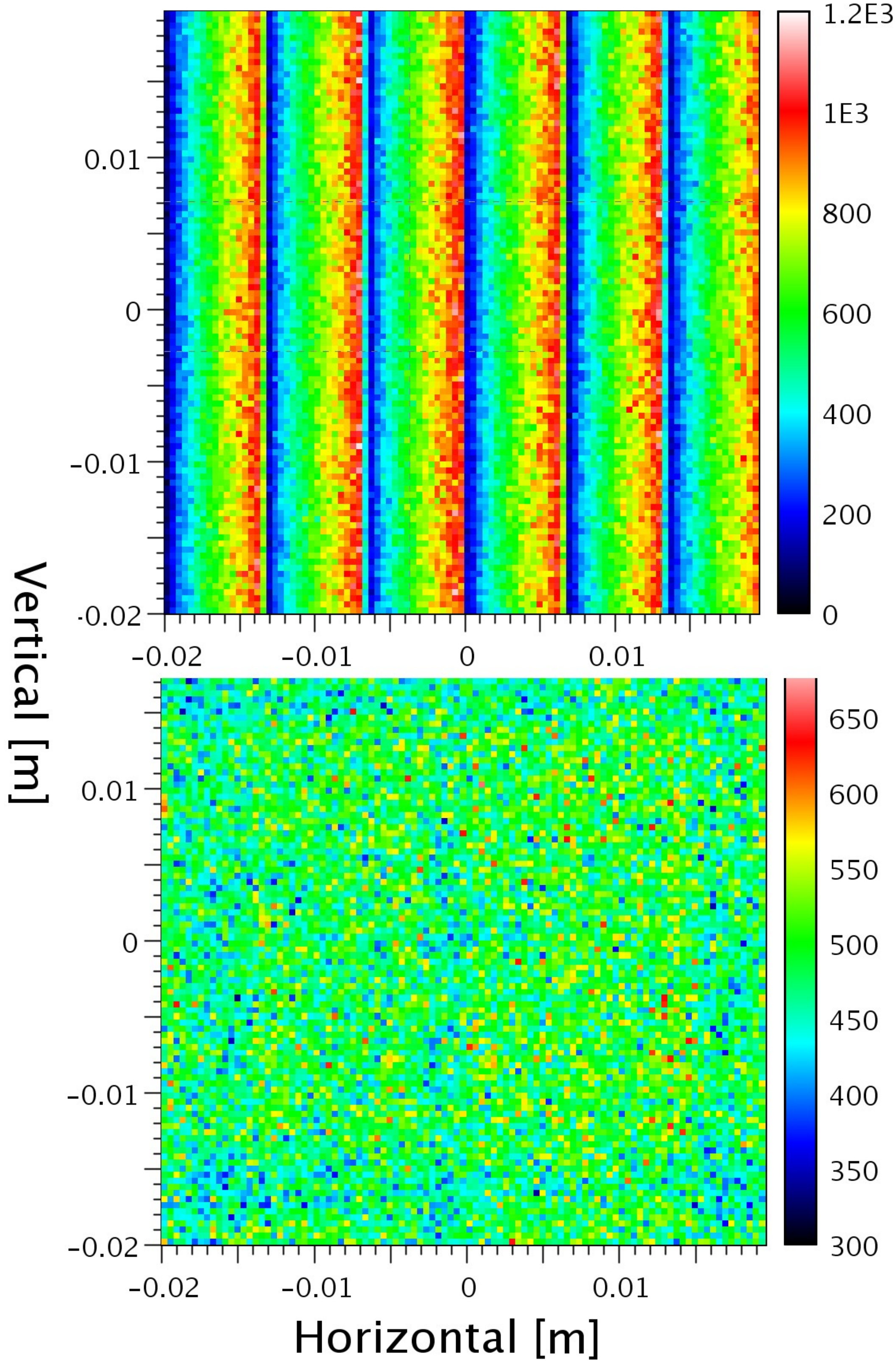
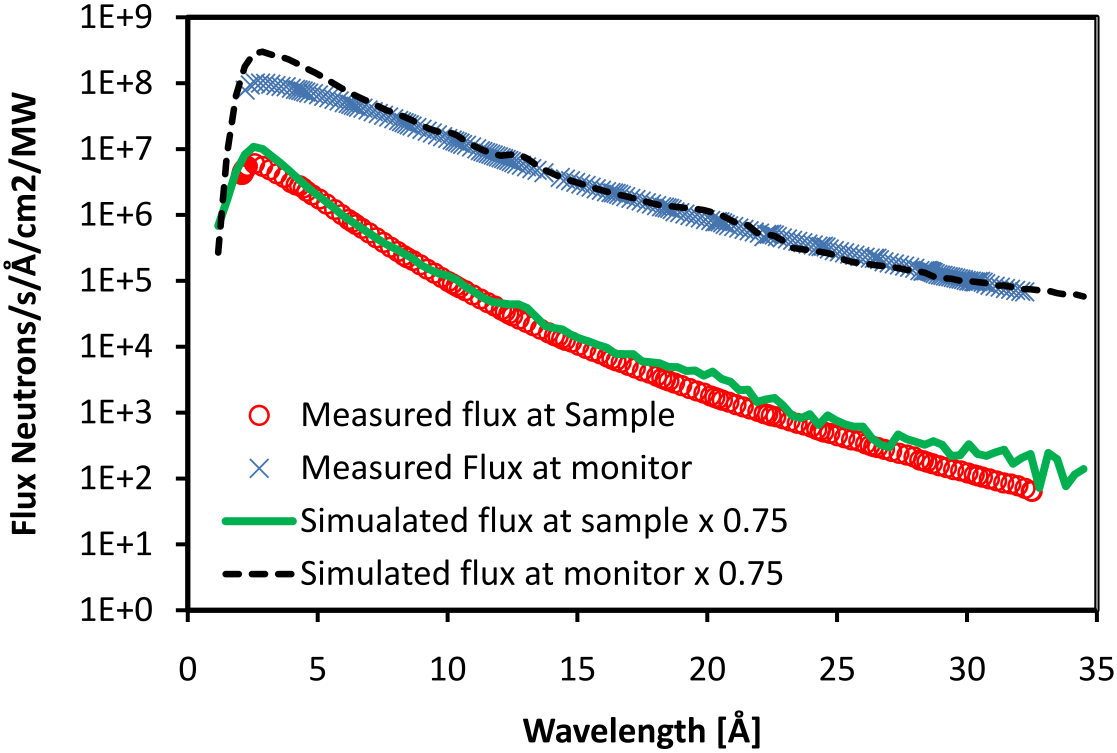

2.85
2.8
2.75
2.7
2.65
2.6
2.55
2.5
Flux On Sample [X10⁶ n/s/cm²/Å
Integrated Flux (2-10Å)
40
60
80
100
120
Guide Height [mm]

Fig 8



1.2E3
1E3
800
600
400
200
0
0.01
0
-0.01
-0.02
-0.02
-0.01
0
0.01
Vertical [m]
650
600
550
500
450
400
350
300
0.01
0
-0.01
-0.02
-0.02
-0.01
0
0.01
Horizontal [m]

Fig 9


1E+9
1E+8
1E+7
1E+6
1E+5
1E+4
1E+3
1E+2
1E+1
1E+0
Flux Neutrons/s/Å/cm2/MW
0
5
10
15
20
25
30
35
Wavelength [Å]
Measured flux at Sample
Measured Flux at monitor
Simulated flux at sample x 0.75
Simulated flux at monitor x 0.75