Montel optics: Tailoring phase-space in neutron beam extraction

S. Weichselbaumer¹, G. Brandl¹², R. Georgii¹², J. Stahn³, T. Panzer⁴, P. Böhn¹

¹Heinz Maier-Leibnitz Zentrum und Physik-Department E21, Technische Universität München, Lichtenbergstr. 1, D-85748 Garching, Germany
²Physik-Department E21, Technische Universität München, James-Franck-Str. 1, D-85748 Garching, Germany
³Laboratory for Neutron Scattering, Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland
⁴Material Science and Simulations, Neutrons and Muons, Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland

Abstract

In view of the trend towards smaller samples and experiments under extreme conditions it is important to deliver small and homogeneous neutron beams to the sample area. For this purpose, Montel mirrors are ideally suited as the phase space of the neutrons can be defined far away from the sample. Therefore, only the useful neutrons will arrive at the sample position leading to a very low background. We demonstrate the ease of designing neutron transport systems using simple analytic tools, which are verified using Monte-Carlo simulations that allow to take into account effects of gravitation and finite beam size. It is shown that a significant part of the brilliance can be transferred from the moderator to the sample. Our results may have a serious impact on the design of instruments at spallation sources such as the European Spallation Source (ESS) in Lund, Sweden.

Keywords: Neutron scattering, European Spallation Source, Neutron guides, Elliptic guides, Montel mirrors, Supermirror, Monte-Carlo simulations, McStas

1. Introduction

Ground-breaking for the European Spallation Source (ESS) in Lund, Sweden is currently planned for summer 2014. ESS is intended to operate at a power of 5 MW and will use a long-pulse moderation for the neutron production. The resulting, time-integrated flux will be comparable to the continuous flux at the high flux reactor HFR at the Institut Laue-Langevin in Grenoble [1]. The peak flux at ESS will exceed the time-averaged flux of the ILL by approximately a factor of 30. Therefore, using time-of-flight techniques the performance will be largely increased. Further increases will be possible by implementing modern neutron transport systems based on non-linearly tapered neutron guides and a clever design of the instruments.

Traditionally, beam lines for neutron scattering and imaging are designed using Monte-Carlo simulations covering a large range of parameter space [2, 3]. As only numerical data is available it is difficult to identify the origin of loss mechanisms during the transport of the neutrons, the influence of various components on the homogeneity of the phase space of the transported neutrons, and maybe most importantly to obtain a clue about the origin of the background at the sample position as the geometrical path of the neutrons is somehow hidden in the huge amount of data sets obtained from the simulations.

For more than three decades, with the invention of neutron guides by Maier-Leibnitz [4], neutrons were transported over large distances mostly by Ni-coated, straight or curved guide tubes. However, due to the small critical angle of total reflection given by \( \theta_c = \frac{m \pi}{\lambda} \), where \( m = 1 \) for Ni, the transport was only efficient for cold neutrons. Using supermirror coatings, the index \( m \) was increased up to \( m = 7 \) [5] thus allowing to even transport epithermal neutrons at spallation sources.

Due to the many internal reflections of the neutrons in straight neutron guides, however, the transmission is seriously reduced [6]. Moreover, the significant losses require massive shielding of the neutron guides. In 2004 Schanzer et al. [7] proposed the use of elliptic neutron guides which reduce the number of reflections to essentially two if the guide is properly designed. Please note that the expression "elliptic guide" is often used for a kind of a "ballistic elliptic guide", which transports the neutrons using many reflections without using a true focusing in terms of the point to point imaging provided by an ellipse in mathematics [8]. For example, the replacement of the straight neutron guide at the beam line HRPD at ISIS by a 90 m long elliptic guide increased the neutron flux at the sample by up to two orders of magnitude [9]. In addition, as the beam paths can be simply identified using geometrical optics, it is straightforward to design and judge the performance of elliptic guides [10]. Recently Klenø et al. have shown that approximately 50% to 90% of the brilliance of cold (4.25 Å ≤ \( \lambda \) ≤ 5.75 Å) and thermal (0.75 Å ≤ \( \lambda \) ≤ 2.25 Å) neutrons can be transported from the moderator to the sample using parabolic or elliptic guide geometries [2]. Effects of gravitation were included.

Often, it is argued that elliptic guides are prone to a large background at the sample because there is a direct view to the moderator. However, by inserting beam blockers in the central part of the guide, the line of sight can be effectively interrupted [11] without affecting the homogeneity of the beam. It is correct, that the blocker leads to a hole in the transmitted phase space as pointed out by Zendler et al. [12], however, this hole is very small and swamped by effects of waviness and gravitation.
if real neutron guide systems are considered [10]. The major background of elliptic guides is caused by the fast neutrons that emerge from the neutron source and illuminate the internal surfaces of the guide close to the sample [10]. These neutrons can effectively be stopped by placing two or more elliptic guides in series [11] with the further advantage that effects of halo and coma aberration are reduced. Even beam blockers may become superfluous. The direct line of sight can also be interrupted by gravitational curving of long neutron guides [13].

Amongst the different guide concepts, Montel optics is very promising in delivering neutrons with an excellent signal-to-noise ratio to the sample because the direct line of sight is effectively interrupted. A Montel mirror consists essentially of two elliptic mirrors that are arranged perpendicular to each other, i.e. the optics consists of a "quarter" of an elliptic neutron guide. These mirrors were invented by Montel in 1957 for focusing X-rays [14] and have now become an integral part of many beam lines at synchrotron sources and for x-ray diffractometers. Recently, Montel mirrors have been used by G. Ice for the focusing of neutron beams [15]. Stahn et al. use them for reflectometry, i.e. for the SELENE project [16]. In addition, a guide system based on Montel mirrors was optimized for a proposed MIEZE type spin echo spectrometer for the ESS [17].

Montel mirrors have many advantages when compared with other concepts for neutron guides. Beside of the advantage of tailoring the neutron beam more than typically ten meters away from the sample position [18], the path of the neutrons through the optical system is readily clear, i.e. it takes place via two reflections in each device. Moreover, the brilliance transfer can easily be evaluated based on reflectivity data of the supermirrors. One drawback of Montel mirrors is the scaling of the length of the mirrors with the beam size. In order to obtain a beam with a diameter of approximately 10 mm, the required distance between the two focal points A and B has to be approximately 20 m.

The aim of the present work is, firstly, to evaluate the performance of various types of neutron guides, including elliptic, Montel and straight guide systems, using geometrical optics and analytical tools (Fig. 1). In a second step we will verify the analytic results using the Monte-Carlo simulation package McStas [19]. Finally, gravitational effects will be taken into account. The results show that it is indeed possible to calculate the performance rather accurately using analytic means.

In order to compare the systems we consider sample sizes \( a \times a \) with 1 mm \( \leq a \leq 20 \) mm. The divergence at the sample is assumed to be 2\(^\circ\) (FWHM). A wide, flat wavelength spectrum 1 Å \( \leq \lambda \leq 15 \) Å will be considered. An aperture with an opening corresponding to the assumed sample size is placed 2 meters away from the moderator for the elliptic and Montel optics (Fig. 1). For the straight guide a cross section of 100 \( \times \) 100 mm\(^2\) and no entry slit is assumed.

2. Analytical calculation without gravitation

In a first step we calculate the angle of reflection of neutrons emerging from a point source at the first focal point \( A \) of the ellipse, hitting the mirror at the point \( P \) and arriving at the second focal point \( B \) (Fig. 2). If the contour of the ellipse is represented by a parametric equation in polar coordinates, the distance \( r \) is given by

\[
AP = r(\theta) = \frac{a(1-e^2)}{1-e \cos \theta}
\]

where \( e = L/2a \) is the numerical eccentricity of the ellipse, \( L = \sqrt{a^2 - b^2} \) is the distance between the focal points \( A \) and \( B \), and \( a \) and \( b \) are the half axes of the ellipse. The local angle of reflection, \( \gamma \), is given by

\[
\gamma = \frac{\pi}{2} - \frac{\alpha + \beta}{2},
\]

(2)

where

\[
a = \frac{\pi}{2} - \theta, \quad \beta = \arccos \left( \frac{r \sin \theta}{2a - r} \right).
\]

(3)

\( \gamma \) can then be used to calculate the reflectivity \( R(\lambda, \gamma) \) of the supermirror in dependence of the neutron wavelength \( \lambda \) and eventually the transmitted intensity can be determined for all wavelengths.

In the following, a point-like source and \( m = 3 \) and \( m = 7 \) supermirror is assumed for the elliptic guide and the Montel mirrors, respectively. The reflectivity profile of the supermirror is parametrized by assuming a constant reflectivity \( R = 1 \) up to a critical value \( Q_c = 0.0219 \frac{\text{Å}}{\text{m}} \) (corresponding to \( m = 1 \)) followed by a linear decrease to \( R = 0.88 \) at \( q = 3Q_c \) and \( R = 0.5 \) at \( q = 7Q_c \) for supermirror \( m = 3 \) and \( m = 7 \), respectively. The transmitted neutron intensity can be determined for all \( \lambda \) by integrating the reflectivity along the whole mirror:

\[
R(\lambda) = \frac{1}{\theta_1 - \theta_0} \int_{\theta_0}^{\theta_1} R(\lambda, \gamma) \, d\theta.
\]

(4)
where \( \theta_0 \) and \( \theta_1 \) are the angles which define the accepted divergence \( (\theta_1 - \theta_0 = 2^\circ \text{ in this work})\). To obtain the intensity for \( n \) Montel mirrors, the reflectivity has to be taken to the power of \( 2n \) since a neutron is reflected two times by each Montel mirror.

The analytic results are verified by using Monte Carlo simulations choosing for the incident beam a size \( 0.1 \text{ mm} \times 0.1 \text{ mm} \), which is small compared to the dimensions of the mirrors and the assumed sample size. The detector at the sample position has the dimensions \( 0.4 \times 0.4 \text{ mm}^2 \). For comparison, we define the brilliance transfer (BT) similar to Klenø et al. [2] as the ratio of the intensity at the sample to the intensity through the slits at the entrance of the guide system (see Fig. 1). At the entrance, only neutrons with a divergence \( \leq 2^\circ \) are taken into account. This procedure is a rather stringent benchmark. Fig. 3 shows that the Monte Carlo simulations match the analytical predictions very nicely. The elliptic guide system shows a BT of 100% even for smaller wavelengths. The reason is that the neutrons are reflected from 4 sides. Therefore, the radii of curvature can be enlarged when compared to Montel mirrors.

As the Monte-Carlo simulations are rather sensitive to the exact position of the guide with respect to the focal points \( A \) and \( B \) of the ellipses the analytical calculations are much more robust and less time consuming. Therefore, whenever possible, analytical calculations for the design of neutron guides should be conducted first to provide a first clue about the possible gains in neutron intensity using various designs. However, to include the effects of a finite moderator size (or entrance slit) and sample size, Monte-Carlo simulations are required.

Fig. 4 shows the BT of the guides for various sizes of the beam defining aperture at the focal point \( A \) of the guide system. The dimensions of the aperture are given in the legend of the figure. At the sample position a detector large enough to capture all transported neutrons was chosen. With increasing beam size the BT decreases as expected due to the effects of halo and coma aberration. These effects lead to a reduction of the BT because they become already effective before the neutrons enter the second Montel mirror system. Fig. 4 shows a kind of best case scenario as the detector collects all transported neutrons going through the guide system. When only neutrons hitting the sample are considered a smaller BT is obtained. For large sample sizes the reduction of the BT is explained by the effects of halo and coma aberration as explained above. Even for a beam size of \( 20 \text{ mm} \times 20 \text{ mm} \), a BT of more than 70% is obtained.

![Figure 2: Schematic view of an elliptic mirror.](image)

Figure 2: Schematic view of an elliptic mirror. \( a \) and \( b \) are the semi-major and semi-minor axis, respectively. \( L \) is the distance between the focal points \( A \) and \( B \). The angles \( \alpha \) and \( \beta \) can be calculated to calculate the reflection angle \( \gamma \) of the neutron trajectory with the surface of the ellipse at the point \( P \).

![Figure 3: Comparison of the BT of a 2× elliptic guide system (\( m = 3.0 \)) and a 2×, 4× and 8× Montel mirror system (\( m = 7.0 \)) versus wavelength.](image)

Figure 3: Comparison of the BT of a 2× elliptic guide system (\( m = 3.0 \)) and a 2×, 4× and 8× Montel mirror system (\( m = 7.0 \)) versus wavelength. The solid lines are the analytically calculated curves and the data points are the result of a Monte-Carlo simulation. The simulations where performed without taking effects of gravitation into account. The opening of the entry slit is 0.1×0.1 mm\(^2\).

![Figure 4: Comparison of the analytical calculation with Monte-Carlo simulations of a two-fold Montel mirror system for different beam sizes.](image)

Figure 4: Comparison of the analytical calculation with Monte-Carlo simulations of a two-fold Montel mirror system for different beam sizes. Shown here is the BT for the neutrons transported from the entrance slit (its size is given in the legend) to the sample position, where a large detector (200×200 mm\(^2\)) is placed to collect all transported neutrons through the guide system. Effects of gravitation are not taken into account.

3. Inclusion of effects of gravitation

In the following we investigate the effect of gravitation on the performance of the transport systems discussed above. Gravitational effects are large. For example, neutrons with \( \lambda = 5 \text{ Å} \) drop 193 mm along a free flight path of 156 m. Due to the complexity of the problem, Monte-Carlo simulations are mandatory. A quantitative comparison of the brilliance transfer (BT) for various \( n \) is shown in Fig. 5 for an aperture of 2×2 mm\(^2\). The dual ellipse system provides a BT of about 45% for \( \lambda \approx 2 \text{ Å} \). For guides composed of Montel mirrors, the maximum of the
BT shifts with increasing $n$ to longer wavelengths because they suffer more under gravitation. For an 8-fold Montel system, the distance between two reflections is approximately 4 times smaller than for a 2-fold Montel system. Therefore, neutrons with large $\lambda$ are transported more efficiently. Of course, if the entrance slit is relaxed the conditions for beam transport will become more favourable and the BT will increase. Actually, it is gratifying that gravitation has not even larger effects on the BT for the small beam size being used.

A detailed analysis of the BT for elliptic guides has been performed by Klenø et al. [2]. They obtain a significantly larger BT at $\lambda = 1.5$ Å and $\lambda = 5.0$ Å due to the following reasons: i) Only one elliptic guide was considered, therefore no neutrons are lost due to the phase space mismatch between the individual guides considered in our model, ii) elliptic guides are less sensitive to gravitational effects in particular for large $\lambda$, and iii) Klenø et al. assumed a rather large beam size of 10 mm × 10 mm.

Fig. 6 shows the performance of the 2-fold Montel system versus sample size with gravitation enabled. The maximum BT is obtained for a sample size of approximately 10 × 10 mm$^2$. The width of the wavelength band $\Delta \lambda/\lambda$ increases from ≈ 0.56 to ≈ 1.2 when the sample size is increased from 1 mm × 1 mm to 20 mm × 20 mm. Despite the large effects due to gravitation, an impressive BT of approximately 40% is achieved around 4 Å and a large sample size. The optimum is obtained for samples 5 × 5 mm$^2$ and 2 Å ≤ $\lambda$ ≤ 6 Å, a parameter range that will be discussed in more detail in the following.

We consider the beam profile of a 2-fold Montel system for 2 Å ≤ $\lambda$ ≤ 6 Å in more detail. It will be of great interest for many instrument designs for the ESS [20]. The results are compared in Fig. 7 a) and b) without and with gravitation for the Montel systems, respectively, and in c) for a straight guide. The aperture size was 5 × 5 mm$^2$. The maximal intensity in Fig. 7 a) is normalized to 100. The maximum intensity in Fig. 7 b) and c) is scaled to this value. The monitor at the sample position in Fig. 7 a) and b) has a size of 15 × 15 mm$^2$. The assumed sample size of 5 × 5 mm$^2$ is indicated by white rectangles. Neutrons may not hit the sample i) due to reflection losses or ii) due to arriving outside the white rectangles thus contributing to the background. The integrated intensity on the sample for the different configurations is shown in table 1.

One can clearly see the effects of an increasing number of mirrors. Two mirror systems lead to an illumination of a large sample area whereas the 8-fold optics leads to a smaller beam spot as the beam size scales with the length of the mirrors. With enabled gravitation the 2-fold and the 4-fold Montel systems provide the best performance. The 8-fold Montel system has a smaller loss due to gravitation effects, however, the reflectivity losses become significant. The double-elliptic guide system suffers from gravitational effects: The beam decreases in size and in intensity. The integrated intensity on the sample decreases by a factor of 2.7.

Gravitation has no effect on the performance of straight guides (table 1) as it only leads to slightly larger angles of reflection for neutrons when they are "hopping" along the guide. The major disadvantage of a straight guide is (beside the reflection losses) the illumination of the surroundings close to the sample thus increasing the background and reducing the signal-to-noise ratio (c.f. Fig. 7 c). Using elliptic guides, most neutrons arrive at the sample. The overall background is low compared to the straight guide.

Finally, we have investigated if the BT can be increased by vertically tilting the second Montel mirror of the two-fold Montel mirror system when gravitation is enabled. It turns out, that the overall number of transported neutron increases for tilting angles up to 0.5°, but actually the beam spot is less well defined as for the case without tilting, leading to a lower BT as less neutrons are hitting the sample.

Of course, if only neutrons within a narrow wavelength band...
have to be transported the effects of gravitation can be compensated by adjusting the profile of the top/bottom sides of the Montel mirrors or elliptic guides leading to a BT close to 100% as shown in Figs. 3 and 4. One may consider the possibility using adaptive optics to optimize the guide shape for the required wavelength range.

4. Conclusions

We have shown that multiple elliptic guides and Montel mirror systems provide an efficient neutron transport from the moderator to the sample. As the selection of the phase space is conducted close to the moderator, the background outside the biological shielding of the neutron source is massively reduced leading to low costs for shielding. Using geometrical optics the brilliance transfer (BT) can be easily calculated if beam size and gravitational effects are neglected, which is possible for short guide systems. Monte-Carlo simulations show that for the assumed unfavorable conditions we considered, i.e. long flight paths of 158 m, large bandwidth, and sample size (as small as a few mm) lead to BTs of 40% or more. If the wavelength band is, however, restricted the horizontal mirror surfaces of the reflecting optics can be adapted in order to reduce or even cancel the effects of gravitation leading to BTs close to 100%.

To transport a similar phase space as elliptic guides, the m-value of the coatings for Montel mirrors has to be increased by a factor of at least two. While 8-fold Montel systems suffer less from gravitation than 1- or 2-fold systems, the BT for small wavelengths is seriously reduced for n = 8. Most likely it is best to realize a guide system consisting of two Montel mirrors only and to adapt the systems such that they take gravitation into account, possibly using adaptive systems that can be used to optimize the transport for a particular wavelength band.

For highest throughput of beams with large divergence and low background, a double elliptic guide system may be the optimum choice. Finally, when choosing the optimum guide geometry the perfection of the mirrors should be respected. Presently, Montel mirrors and neutron guides have a waviness of \( \approx 1.0 \cdot 10^{-5} \) rad and \( \approx 1.0 \cdot 10^{-4} \) rad, respectively, leading to a blurring of the beam over a distance of 100 m of 1 mm and 10 mm, respectively. These values should be compared with the effects of gravitation.

In a further study one may also consider more advanced geometries for Montel optics such as systems being composed of parabolic Montel mirrors at the entrance and the exit of a guide system connected via a long straight guide section. Such a geometry may reduce the effects of gravitation further.

In the future, it may become possible to build neutron sources based on the ejection of photo neutrons from halo isomers by means of \( \gamma \) - and laser beams, which will provide neutron beams with a very high brilliance [21] and a small diameter of the order of 0.1 mm. The small beam size leads to short mirrors and therefore effects of gravitation become a minor issue.

| Instrument   | No gravity | Gravity | Ratio |
|--------------|------------|---------|-------|
| 2\( \times \) Ellipse | 47.1       | 17.7    | 2.66  |
| 2\( \times \) Montel | 62.5       | 25.6    | 2.44  |
| 4\( \times \) Montel | 41.3       | 26.5    | 1.55  |
| 8\( \times \) Montel | 19.6       | 17.1    | 1.15  |
| Straight Guide | 39.3       | 39.3    | 1.00  |

Table 1: Integrated intensities on a 5 \( \times \) 5 mm\(^2\) sample for a wavelength band of 2 Å–6 Å for the different configurations. The unit is \( 10^9 \) neutrons/cm\(^2\) /s. A ratio close to 1 means that gravitation has only a small effect on the transport properties.
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