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# Tailoring phase-space in neutron beam extraction

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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, elliptic and/or 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 numeric tools, which are verified using Monte-Carlo simulations that allow taking into account effects of gravity 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.

## 1. Introduction

The foundation laying for the European Spallation Source (ESS) in Lund, Sweden took place in October 2014. ESS is intended to operate at a power of 5 MW and will use a long-pulse target station for the neutron production. The resulting time-integrated flux will be comparable or even larger than the continuous flux at the high flux reactor (HFR) at the Institut Laue-Langevin in Grenoble [1]. However, the peak flux at ESS will exceed the time-averaged flux of the ILL by at least 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.

For more than three decades, with the invention of neutron guides by Maier-Leibnitz and Springer [2], 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 $\theta/^\circ = 0.099\,m\lambda/\AA$, where $m=1$ for Ni, the transport was only efficient for cold neutrons. Using supermirror coatings, the index $m$ was increased up to $m=7$ [3] thus allowing to even transporting epithermal neutrons with wavelength of 1 Å at spallation sources.

Due to the many internal reflections of the neutrons in straight high-$m$ neutron guides, however, the transmission is seriously reduced [4]. Moreover, the significant losses require massive shielding of the neutron guides. Mezei [5] and Schanzer et al. [6] proposed the use of ballistic and truly bent elliptic neutron guides, respectively, which reduce the number of reflections significantly. Elliptic guides are focusing the neutrons from the moderator exit to the sample in terms of the point to point imaging provided by an ellipse in mathematics [7]. 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 [8]. 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 [9]. Recently Klenø et al. have shown that approximately 50–90% of the brilliance of cold $(4.25\,\AA \le \lambda \le 5.75\,\AA)$ and thermal $(0.75\,\AA \le \lambda \le 2.25\,\AA)$ neutrons can be transported from the moderator to the sample using parabolic or elliptic guide geometries [10]. Effects of gravity were included in this study.

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]. 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, as for instance in our simulation of the order of 0.12 (see Fig. 7b). The major background of elliptic guides is caused by the fast neutrons that emerge from the neutron source and

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illuminate the internal surfaces of the guide close to the sample [9]. 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, if an even number of guides is used. Then 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 other guide concepts, Montel guides are very promising in delivering neutrons to the sample. 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 *x*-ray diffractometers. Recently, Montel mirrors have been used by 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].

A Montel mirror consists of two elliptic mirrors that are arranged perpendicular to each other, i.e. the optics consists of half of a four-sided elliptic neutron guide. In the center of the Montel mirror a beamstop can be placed for defining the accepted divergence independent from the beam size which is defined by the entrance aperture. Because the Montel mirror is inclined in the horizontal and vertical directions the direct line of sight is interrupted leading to an excellent signal-to-noise ratio on the sample.

Montel mirrors have many advantages when compared with other concepts for neutron guides. Besides the advantage of tailoring the neutron beam more than typically 10 m away from the sample position [18], the path of the neutrons through the optical system is 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.

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 numeric results using the Monte-Carlo simulation package McStas [19]. The results show that it is indeed possible to calculate the performance for small beam and sample sizes and ignoring gravity rather accurately using simple analytical means. Finally, gravitational effects will be taken into account using Monte-Carlo simulations.

## 2. Numeric calculations without gravity

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

$$\overline{AP} = r(\theta) = \frac{a(1-e^2)}{1-e\cos\theta} \tag{1}$$

where $e = L/2a$ is the numerical eccentricity of the ellipse, $L = 2\sqrt{a^2-b^2}$ 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

$$\gamma = \frac{\pi}{2} - \frac{\alpha+\beta}{2} \tag{2}$$

where

$$\alpha = \frac{\pi}{2} - \theta, \quad \beta = \arccos\left(\frac{r\sin\theta}{2a-r}\right). \tag{3}$$

$\gamma$ 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 a $m=7$ supermirror (which is currently state-of-the-art) is assumed for all guides. The reflectivity profile of the supermirror is parametrized by assuming a constant reflectivity $R=1$ up to a critical value $Q_c = 0.0219\,^{\circ}\mathrm{A}^{-1}$ (corresponding to $m=1$) followed by a linear decrease to $R=0.5$ at $q = m\cdot Q_c = 7Q_c$. The transmitted neutron intensity for a specific wavelength can be determined by integrating the reflectivity along the whole mirror:

$$R(\lambda) = \frac{1}{\theta_1-\theta_0}\int_{\theta_0}^{\theta_1} R'(\lambda,\theta)\,\mathrm{d}\theta \tag{4}$$

where $\theta_0 = \arctan(w/(L-l_{\text{in}}))$ and $\theta_1 = \arctan(w/l_{\text{in}})$ (see Fig. 2) are the angles which define the accepted divergence. $w$ and $l_{\text{in}}$ are the distance of the guide to the central axis and the distance between the focal point to the guide entry, respectively. To obtain the intensity for $n$ Montel mirrors, the reflectivity has to be taken to the power of $2n$ since a neutron is reflected twice by each Montel mirror.

The numeric results are valid in the limit of a vanishing sample size when compared with the dimensions of the guide. Therefore we verified the results by using Monte Carlo simulations choosing for the in and outgoing beam a size $5\times5\,\mathrm{mm}^2$ with a small divergence of 0.25° (FWHM). To compare the different guide concepts we use the brilliance transfer (BT) as it was defined by Klenø et al. [10]. The brilliance or phase space density $\Psi$ is the number of neutrons per unit time, area, solid angle and wavelength interval. According to Liouville's theorem the brilliance transfer $\mathrm{BT} = \Psi_{sample}/\Psi_{entry}$ can never be larger than one. To measure the BT we place monitors with the same restriction in size, wavelength and divergence after the entry slit (for the straight guide in front of the guide entry) and at the sample position.

Fig. 3 shows that the Monte Carlo simulations match the functional form of the numeric predictions very nicely and predict in the case of the Montel optics even correctly the BT. The smaller than predicted BT for the elliptic guides can be attributed to the absorption of neutrons in the beam stop in the elliptic guides which is not included in the analytical model. Due to the small divergence used this effect is particularly strong in Fig. 3 and will be less prominent in the simulations with larger divergence of 1° (FWHM) which will be used in the following section.

In the light of these results, whenever possible, numeric calculations for the design of neutron guides should be conducted first to provide independent tests of the correct placement of the guides in the simulations. It allows also for first estimations of the efficiency of a neutron guide system facilitating and speeding up the comparison of different designs. However, to include the effects of larger beam and sample sizes and the effect of gravity Monte-Carlo simulations are required.

## 3. Inclusion of effects of gravity

In the following we investigate the effect of gravity on the performance of the transport systems discussed above. Gravitational effects are large: For example, neutrons with $\lambda = 5\,^{\circ}\mathrm{A}$ drop 193 mm along a free flight path of 156 m. Due to the complexity of the problem, Monte-Carlo simulations are mandatory.

For all simulations in this section a flat wavelength spectrum with a brilliance of $\Psi = 1\times10^{12}\,\mathrm{cm}^{-2}\,\mathrm{s}^{-1}\,^{\circ}\mathrm{A}^{-1}\,\mathrm{sterad}^{-1}$ for $1\,^{\circ}\mathrm{A} \le \lambda \le 15\,^{\circ}\mathrm{A}$ is considered. The divergence at the sample is assumed to be 1° (FWHM). An aperture with an opening corresponding to the assumed sample size is placed at the position of the closest place for a neutron guide at the ESS, i.e. 2 m away from the moderator (see Fig. 1). For the straight guide a cross-section of