

Neutron optics concept for the materials engineering diffractometer at the ESS

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Abstract. The Beamline for European Materials Engineering Research (BEER) has been recently proposed to be built at the European Spallation Source (ESS). The presented concept of neutron delivery optics for this instrument addresses the problems of bi-spectral beam extraction from a small moderator, optimization of neutron guides profile for long-range neutron transport and focusing at the sample under various constraints. They include free space before and after the guides, a narrow guide section with gaps for choppers, closing of direct line of sight and cost reduction by optimization of the guides cross-section and coating. A system of slits and exchangeable focusing optics is proposed in order to match various wavelength resolution options provided by the pulse shaping and modulation choppers, which permits to efficiently trade resolution for intensity in a wide range. Simulated performance characteristics such as brilliance transfer ratio are complemented by the analysis of the histories of “useful” neutrons obtained by back tracing neutrons hitting the sample, which helps to optimize some of the neutron guide parameters such as supermirror coating.

1. Introduction

The long pulse concept of the European Spallation Source (ESS) brings about new challenges for the design of neutron scattering instruments. While other spallation sources provide sufficiently short pulses which can be directly used for wavelength definition, the 2.86 ms long pulse of the ESS needs to be further tailored in most cases in order to achieve sufficient resolution. It is particularly the case of diffraction experiments, where the relative wavelength resolution $\Delta\lambda/\lambda$ below 1% must be achieved at short wavelengths. This leads to an increased complexity and cost of such instruments due to the installation of choppers for pulse shaping. On the other hand, instruments at ESS can profit from the pulse tailoring as it permits to adjust instrument resolution to a particular problem. This feature can bring significant advantage over the short pulse sources, where the pulse width and its dependence on the wavelength is determined by the moderator and the possibility to trade resolution for intensity is limited to adjusting beam divergence [1-3]. However, the possibility of choosing wavelength resolution does not provide more flexibility by itself, it has to be accompanied by properly designed neutron optics which allows to match the beam properties, especially the divergence, to the wavelength resolution.



This paper introduces the concept of neutron delivery optics for the diffractometer BEER (Beamline for European materials Engineering Research) at ESS, which allows for such a flexibility. It is a 159 m long time-of-flight (ToF) powder diffractometer that has been proposed to address the needs of materials engineers from both academic and industrial areas. It will provide new capacity for in-situ and in-operando studies of materials under external conditions, which are relevant for materials production, treatment and use, but also in the traditional domain of residual strain mapping. In addition, optional measurements of small-angle scattering (SANS) and direct imaging are envisaged [4]. This broad scale of techniques calls particularly for the above mentioned adaptability of neutron optics. The required quantitative characteristics of the neutron beam in the main operation modes are derived in Section 2, which is followed by the description of the main components of the neutron transport system (Section 3). Section 4 then summarizes the performance of the system in terms of brilliance transfer efficiency.

2. Required neutron beam characteristics

Regarding the neutron beam properties, the main criteria for an engineering diffractometer are the wavelength resolution and bandwidth, gauge volume size and angular divergence. The neutron transport system can be well characterized by the quantity called brilliance transfer (BT) ratio defined as the neutron intensity integrated over a pre-defined beam area, solid angle and wavelength interval, relative to the source brightness. Due to the Liouville's theorem, BT ratio ≤ 1 . It describes the quality of the neutron delivery optics alone, regardless of the source spectrum. It is however important to define the integration intervals adequately with respect to the assumed mode of operation. In addition, qualitative criteria such as uniformity of angular distribution should be considered.

2.1. Wavelength

While it is relatively easy to transport cold neutrons, the short wavelength limit is critical for the design of neutron guides. In contrast to general purpose powder diffractometers, experiments at an engineering diffractometer are usually carried out on materials with known crystallographic structure of main constituting phases. This partly relieves the requirements on wavelength bandwidth since a smaller set of reflections is required for Rietveld analysis to yield data on phase composition, lattice strain or texture compared to full structure refinement. From this point of view, the BT ratio close to the lower wavelength limit of $\lambda \geq 1 \text{ \AA}$ is a suitable figure of merit for optimizations. Although the instrument can operate below 1 \AA , its performance there can be traded for other important characteristics without significant impact on the scientific output. On the other hand, delivery of cold neutrons up to $\lambda \cong 6 \text{ \AA}$ or more is also needed in order to be able to measure diffraction in transmission mode (Bragg edge), to increase contrast for imaging experiments and to reach suitable momentum transfer range for SANS. Therefore, a bi-spectral extraction optics has to be incorporated into the neutron guide feeder.

2.2. Gauge volume

The required beam area varies significantly according to the experiment type. It may be very small (below 1 mm^2) in the case of residual strain mapping, but also rather large in the case of in-situ experiments (typically $5 \times 10 \text{ mm}^2$). The latter value has been chosen as the integration interval for BT evaluation since this is the typical operation mode assumed at BEER.

2.3. Trading resolution for intensity

Tuning of the beam divergence with respect to the required resolution in lattice parameter, $\Delta d/d$ is assumed for the reasons explained in Section 1. Relaxing resolution in order to boost the neutron flux is meaningful only if it leads to an increase, or at least conservation, of the overall figure of merit. Whereas various proposals for such a figure of merit in the case of a powder diffractometer can be found in literature, the traditional definition as the *integral intensity over the square of the peak width*,

$$FoM = I \left(\frac{\Delta d}{d} \right)^{-2} \quad (1)$$

is well justified for an engineering diffractometer [5]. The intensity, I is proportional to the phase space volume transported by the neutron guides and choppers from the source, that is to the product of the widths in wavelength, $\Delta\lambda$, horizontal divergence, $\Delta\alpha$, and vertical divergence, $\Delta\beta$,

$$I \propto \Delta\lambda \cdot \Delta\alpha \cdot \Delta\beta . \quad (2)$$

These three components also contribute to the instrument resolution, which can be formally expressed as

$$\left(\frac{\Delta d}{d}\right)^2 \cong \left(\frac{\Delta\lambda}{\lambda}\right)^2 + \left(\frac{\Delta\alpha}{2 \tan \theta}\right)^2 + \left(\frac{h \Delta\beta}{8 L_D \tan \theta}\right)^2 \quad (3)$$

where h and L_D are the detector height and distance, respectively and 2θ is the scattering angle. This equation holds only approximately for 2θ near $\pm 90^\circ$, it neglects other contributions (sample size, detector resolution) and second order effects (aberration), but it still provides a useful guide for the estimation of optimum beam divergences. It is important to note that the widths $\Delta\lambda$, $\Delta\alpha$ and $\Delta\beta$ in the above equations should take into account different distribution functions of the respective variables. They are therefore calculated from the corresponding variances as $\Delta x^2 = 8 \ln 2 [\langle x^2 \rangle - \langle x \rangle^2]$.

The highest value of the figure of merit is achieved if all the three terms in equation (3) keep approximately the same value. Neutron intensity then increases with the 3rd power of resolution as desired. This condition permits to estimate optimum beam divergences for various settings of the pulse shaping choppers. Examples for three different resolution modes are given in Table 1, where $\Delta\lambda/\lambda$ was calculated from pulse profiles simulated at $\lambda=2 \text{ \AA}$.

Table 1. Wavelength resolutions provided by various chopper settings and corresponding optimum horizontal and vertical divergences.

resolution	$\Delta\lambda/\lambda$ [%]	$\Delta\alpha$ [mrad]	$\Delta\beta$ [mrad]
high	0.08	1.5	12
medium	0.20	4.0	32
low	0.52	10	83

2.4. Constraints

Apart of the beam characteristics given above, the concept of neutron optics must comply with several restrictions. One of them is the free space of 2 m between the source and the guide system entry required due to radiation heating and source design. This is a major obstacle for efficient neutron transport from low dimensional moderators, such as the 30 mm high pancake moderator [6] considered in this work. A similar problem occurs on the opposite side, where the minimum 1 m distance between the guide exit and sample is required in order to provide space for the large sample environment devices planned for BEER. Another limitation arises from the need to install a cascade of choppers in the cavity just after the exit from the target monolith, between 6 and 9.5 m from the source. There, several gaps in the neutron guide have to be provided for the choppers and the beam width is reduced to about 20 mm in order to achieve short transition times. Closing the direct line of sight in order to reduce background arising mainly from fast neutrons is relatively easily achieved by bending of the long neutron guide. However, the high power of the ESS source requires that this closure takes place before one half of the instrument length. This obviously affects the brilliance transport efficiency at short wavelengths. Last, but not least, cost is an important factor for such a long neutron transport system. Significant cost reduction can be achieved by reducing the cross-section of neutron guides and the critical angle of their multilayer coating. Therefore, a trade-off between these parameters and instrument performance has to be an integral part of the conceptual design of neutron guides. The following section shows how all these requirements were incorporated into the neutron optics concept of BEER.

3. Components of the neutron optics system

The initial concept of the instrument has been naturally created on the basis of existing knowledge and experience regarding efficient neutron transport over long distances. Recent studies show that very high BT ratios can be achieved with elliptic guides or ballistic guides with elliptical ends [7-9]. Although an elliptic guide is theoretically an ideal tool for point-to-point focusing, aberration effects strongly influence its real performance already with rather small source and target sizes of few millimetres. Several strategies for reducing the aberration effects have been suggested in literature, such as the double ellipse [10-11] or hybrid elliptic-parabolic guide [12] configurations. However, the extreme eccentricity of the elliptic profile required for neutron transport makes the analytical approach based on a single or double reflection model unusable in many practical situations, especially in the case of long transport distances. Quantitative evaluation of the guide system performance and its optimization therefore requires numerical simulations. The advantage of simulations is not only in the high level of physical reality they can describe, but also in the ability to yield information that can't be obtained by other means, including measurements. Namely, recording of neutron histories during ray-tracing permits to back-trace neutrons that hit the sample and that are thus relevant for an experiment. Analysis of these "useful" neutrons can reveal where they come from, where they get absorbed or reflected etc. We have used this approach to more deeply analyse properties of the proposed neutron optics system and to optimize some of its parameters, such as supermirror coating.

Neutron optics concept for the BEER instrument is therefore based on the ballistic guide geometry with elliptical ends, which was further modified to match the requirements described in Section 2 and optimized by ray-tracing simulations with the program SIMRES [13]. For numerical optimizations by the particle swarm algorithm [14], we have defined the figure of merit as the BT ratio calculated for the beam area $5 \times 10 \text{ mm}^2$ (width \times height) and solid angle $5 \times 30 \text{ mrad}^2$. This choice corresponds to the assumed most usual operation mode with in-situ experiments at the medium resolution (see Table 1). The following sections describe the three main parts of the neutron transport system: (i) beam extraction, (ii) long-range transport and (iii) focusing at the sample. Their configuration was optimized for the ESS pancake source concept [6], assuming 10 cm wide, 3 cm high thermal and cold moderators placed side by side, separated by a 2 cm gap. This concept has been recently replaced by a new "butterfly" configuration, therefore the parameters given in this paper are probably not the final ones to be used in the instrument construction. However, the two moderator geometries are rather similar as for the moderators height and separation and the neutron optics can thus be rather easily adapted to the new geometry without major modification of the presented concept.

3.1. Neutron beam extraction

The beam extraction starts at 2 m from the source by the 4 m long monolith insert, including the bi-spectral multi-mirror optics and neutron guides. It is followed by a 3.5 m long chopper cave where the guide is interrupted by several gaps and the width is reduced to 20 mm. The guide then expands to reach the final cross-section of $40 \times 80 \text{ mm}^2$ at 15.5 m from the source (figure 1a,b). Vertically, the guide profile forms part of a semi-ellipse with the focal distance optimized for the source height of 30 mm.

In the horizontal plane, the feeder is less important as the moderators are sufficiently wide to over-illuminate the 2 cm wide beam port at the exit from the monolith. The acceptance area of this setup fits well the moderator geometry (see figure 1c).

The bi-spectral extraction system proposed for BEER has been studied earlier by C. Zendler et al. [15]. It consists of an array of 8 semi-transparent mirrors on 0.5 mm thick single crystal Si substrate, which transmit thermal neutrons from the thermal moderator, but reflect low-energy neutrons from the cold moderator into the same guide. The length of 0.5 m, supermirror coating with $m=4$ ($m=1$ corresponding to the critical angle of Ni, $0.1^\circ/\text{\AA}$) and inclination angle 0.78° were calculated to match the beam size and the crossover of the cold and thermal spectra at $\lambda_c=1.95 \text{ \AA}$. Given the separation of the moderators, the mirrors have to start at about 4.15 m from the source. Good performance of such a system was predicted by ray-tracing simulations, showing the efficiency between 70 % and 80 % for both thermal and cold neutrons. Note that the "useful" neutrons are extracted from a smaller area on the

cold source (figure 1c) due to the focusing effect of the multi-mirror setup which acts as a Laue lens. This effect would be enhanced if the device can be placed in the middle between the source and the 20 mm beam port.

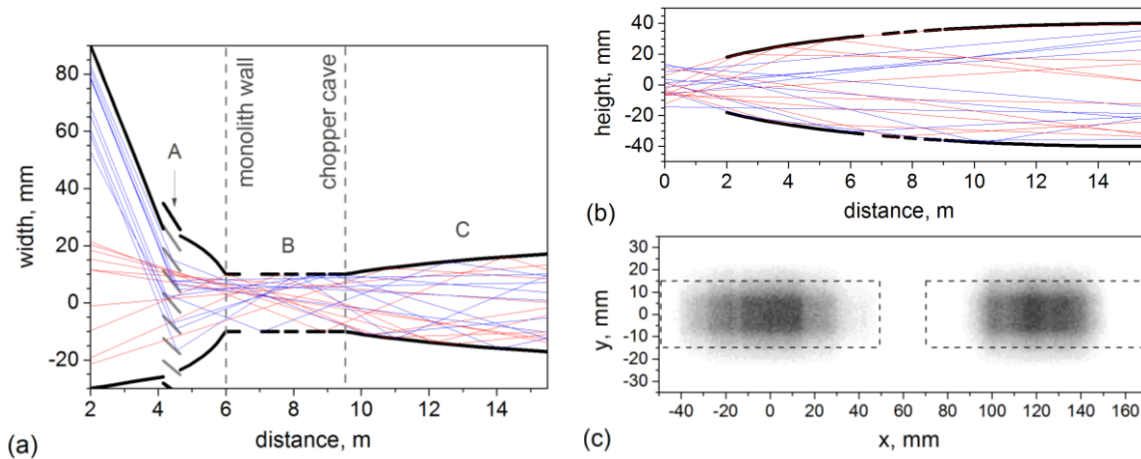


Figure 1. (a) Horizontal profile of the beam extraction including the bi-spectral optics (A), the narrow chopper section (B) and the expanding section (C). (b) Corresponding vertical profile. The thin lines show a sample of neutron trajectories. (c) Acceptance diagram of the guide system represented by the intensity of “useful” neutrons emitted at the source position (the rectangles show the active moderator areas).

3.2. Long-range neutron transport

The long guide spanning the distance between the extraction and focusing sections has to tackle two main problems: (i) transport of a large vertical divergence over the long distance and (ii) closing the direct line of sight for fast particles. Optimization of the vertical profile was carried out in order to minimize the guide height (and therefore cost), while keeping a high BT ratio. It has been modeled by a ballistic guide of the total length $L=154$ m spanning the whole length of the guide system. The focal length, f , of the elliptic ends (practically equal to the major semi-axis length) was taken together with the entry and exit heights as a free parameter for numerical optimization. Resulting BT values as a function of the guide height (minor axis of the ellipse) are plotted in figure 2.

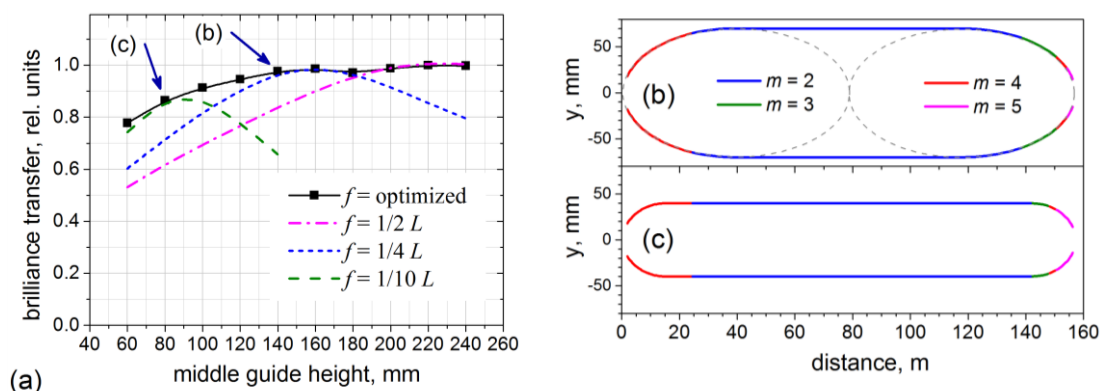


Figure 2. (a) Simulated brilliance transfer ratio as a function of the maximum guide height with optimized (points) and fixed (dashed lines) lengths of the elliptic sections. The arrows point to the two solutions on the right panel. (b) The optimum profile corresponding to a double ellipse. (c) The cost-efficient solution with reduced height.

This result shows that the guide height can be reduced from a full ellipse configuration ($f=L/2$) down to a ballistic profile enveloping a double ellipse, $f=L/4$ (figure 2b) without any loss of transport efficiency. The guide height can be further reduced if a small performance reduction is accepted, leading to the proposed setup with the height of 80 mm (figure 2c) and BT reduction to about 85 % of the maximum. Closing the direct line of sight as close as possible to the source requires a compromise to be made between the guide curvature and transmission of short wavelength neutrons. Figure 3a shows the intensity of illumination of the guide walls by straight rays emitted from the source as simulated by the ray-tracing method. The curvature $1/R > 0.06 \text{ km}^{-1}$ is necessary in order to suppress the direct line of sight before one half of the instrument length. Figure 3b then illustrates that this value is also near the limit of what is acceptable regarding transport efficiency, costing about 8% of brilliance transfer at $\lambda = 1 \text{ \AA}$. The 126 m long parallel guide with cross-section $40 \times 80 \text{ mm}^2$ and curvature 0.06 km^{-1} is therefore proposed for BEER as a cost-efficient solution.

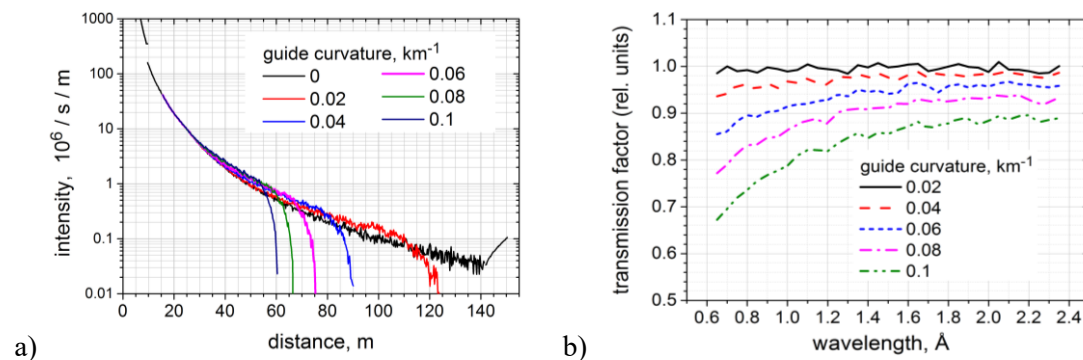


Figure 3. (a) Illumination of the guide walls by direct rays from the source. (b) Decrease of the brilliance transfer ratio due to the guide bending as a function of wavelength.

3.3. Focusing at the sample

After the bent parallel guide, neutrons are focused vertically by a 14.5 m long elliptic guide at the sample, which is placed 1 m after the guide exit leaving thus enough space for large sample environment. The guide width remains constant at 40 mm. This guide is actually divided in 3 sub-sections with the lengths 9 m, 3.5 m and 2 m, respectively (figure 4a).

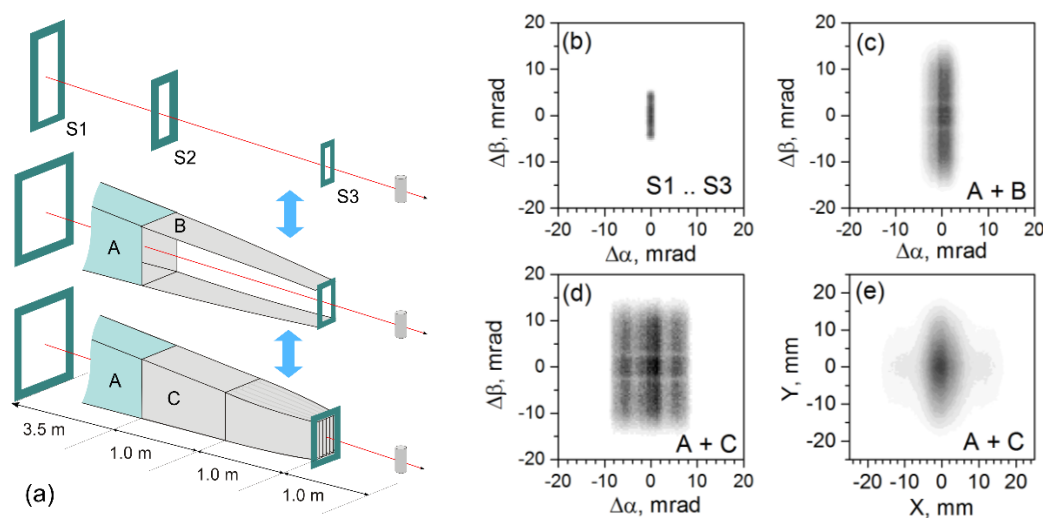


Figure 4. (a) Focusing section with the exchangeable guide segments. (b-d) Divergence distribution at the sample for three resolution modes. (e) Flux distribution at the sample with the horizontally focusing segment.

The last two sections (A,B) are placed in between a pair of adjustable slits (S1 and S3). These guides are removable and can be optionally replaced by another slit (S2) or by another vertically tapered guide, which includes a horizontally focusing multichannel segment (C). This system of three slits (S1-S3) and three guides (A-C) allows to adjust beam divergence in a wide range (figure 4b-e) as required, although the extreme vertical divergence of 83 mrad suitable for low resolution measurements (Table 1) could not be reached.

3.4. Coating optimization

Cost of neutron guides strongly depends on the number of coating layers and hence the critical angle. Recording of neutron histories during ray-tracing permits to calculate statistical distribution of bouncing angles along the guides and thus to find the maximum m value required for the guide coating at given positions. Fig. 5 shows such a distribution recorded for the proposed neutron guide system. In this simulation, $m=5$ was considered on all reflecting walls in order to allow for higher reflecting angles. However, the figure shows that $m=2$ is sufficient for most of the neutron guides length except the initial part of the beam extraction, the chopper cave, and the tip of the focusing guide.

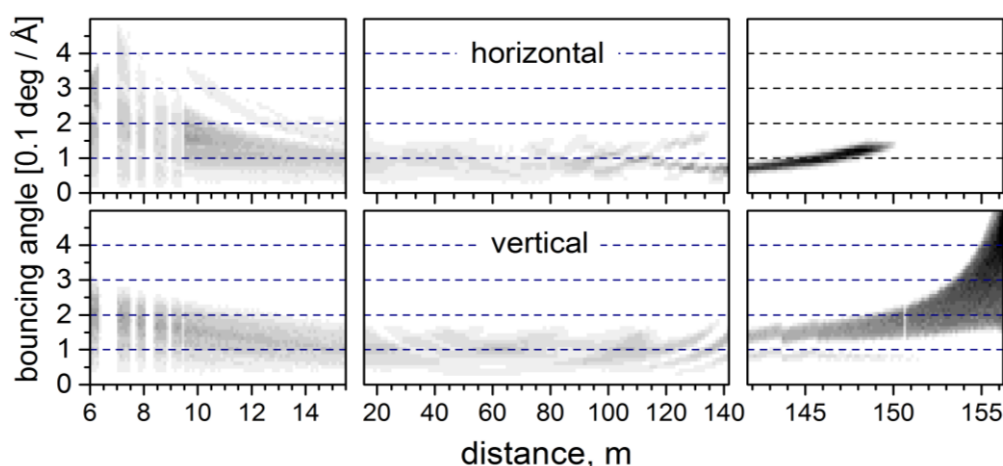


Figure 5. Distribution of bouncing angles along the guides for the left/right (a) and top/bottom (b) mirrors. Only “useful” neutrons that hit the sample are recorded.

4. Summary characteristics

The performance of the neutron guide system described in the preceding section has been assessed by the simulation of the BT ratio as a function of wavelength over the assumed operation range (see figure 6) for the medium resolution mode (see figure 4c) with the target area of $5 \times 10 \text{ mm}^2$ and the acceptance solid angle of $5 \times 30 \text{ mrad}^2$. Physical reality which was taken into account included gravity, Gaussian mirror waviness ($\sigma=0.2 \text{ mrad}$), the sequence of gaps for choppers (figure 1a) and an approximation of the elliptic walls by flat segments with lengths varying from 1 m in the middle section to 0.1 m at the ends. Without the bi-spectral optics, the BT ratio of 50% was achieved for cold neutrons, which then decreased down to 30% at $\lambda=1 \text{ Å}$. The bi-spectral optics add another factor of 70 to 80 % for most of the wavelength range of interest. This is less than one may achieve under ideal conditions [8-9], but closer to the real situation when various constraints imposed by other technologies (e.g. choppers, sample environment) or cost limits have to be taken into account. The loss of BT ratio is mainly due to the non-uniform filling of the phase space (apparent in figure 4), which results from the combination of two factors: (i) small moderator height and the safety distance of 2 m, which do not permit to over-illuminate the entrance port of the neutron guide system, and (ii) choosing less than optimal guide height (see Section 3.2) for cost efficiency.

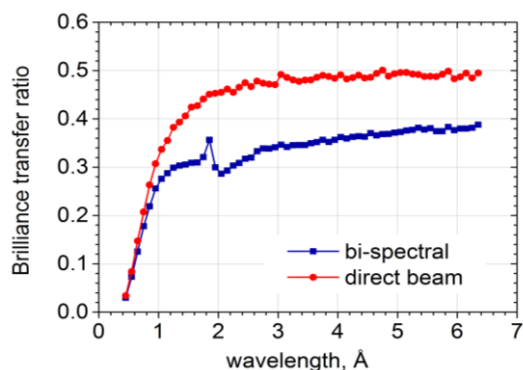


Figure 6. Brilliance transfer ratio for the whole guide system (solid line) and for the direct beam without bi-spectral extraction (guides only, dashed line).

5. Conclusions

The proposed neutron optical system for the BEER instrument addresses successfully most of the instrument requirements and constraints. In particular, it permits to efficiently trade resolution for intensity in a broad range facilitated by the pulse shaping and modulation chopper techniques. The reduced brilliance transfer ratio due to the bi-spectral extraction, small moderator height and other spatial and cost constraints is compensated by the high brightness of the low-dimensional moderator and the outlined instrument flexibility. The neutron optics system is well adapted to other key components of the instrument, such as the chopper system, detectors and specialized sample environment for materials engineering. As the final design of the neutron delivery system for BEER is yet under development, this concept is presented with the prospect of serving as a reference for further modifications improving the instrument performance.

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