Guide design study for the high-resolution backscattering spectrometer FIRES

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Abstract. Different options are considered to transport cold neutrons along 90 m for the proposed new spectrometer FIRES at the ISIS facility. Monte Carlo simulations using the McStas programme package are used to assess the performance of various guide designs from the biological shield to the sample position. By employing a curved geometry, to avoid the direct line of sight, a hybrid design which combines a curved ballistic guide and an elliptic focusing section appears to be the best solution.

1. Introduction
FIRES will be a new high-resolution backscattering spectrometer, proposed for the ISIS facility [1]. It aims to achieve an order of magnitude higher energy resolution compared to the existing near-backscattering spectrometers IRIS and OSIRIS, enabling new measurement possibilities in diverse fields ranging from biopolymers and viscous liquids to hydrogen storage materials and quantum magnets.

To obtain such a high resolution short-time incoming pulses have to be provided and a long flight path is advantageous. One possible approach is to position the instrument on a decoupled or even poisoned moderator. Such a configuration is used at the SNS backscattering spectrometer BASIS [2]. A different solution is to install a chopper to produce short pulses [3]. Furthermore, a pulse-shaping chopper allows changes to the resolution width by altering the incoming pulse width, hence trading resolution against intensity. Such a design has been proposed for the DNA spectrometer at JPARC in Japan [4]. The secondary spectrometer of these high resolution instruments consists of large-area silicon analysers in near backscattering geometry and position-sensitive detectors (psd).

To transport neutrons a long way the ballistic guide idea was proposed [5]. Later nonlinear tapering geometries have been suggested, like parabolic and elliptic geometries [6], which can be combined in various forms [7]. These new geometries combined with new technological developments, which promise supermirror coatings up to $m = 6$ values [8], provide numerous options to design sophisticated guide geometries. The $m$-value defines the factor of critical angle of a supermirror compared to the critical angle of a natural nickel guide.
2. Simulations
A suitable compromise between high intensity and dynamic range proposes a flight path length of about 90 m for the FIRES instrument [1]. We are focusing on the specific layout at ISIS which consists of a distance of 1.7 m from the moderator to the guide entrance and a length inside the biological shield of 4.54 m (see figure 1). Both lengths will not be changed and the guide dimensions \((4.3 \times 6.5)\) cm inside the biological shield will not be varied, only a change of the coating will be considered. To allow for large sample environments, like a high field magnet, at the sample position, a necessary distance of 0.35 m between the end of the guide and sample position was chosen. The FIRES instrument will use a silicon (111) analyser system in backscattering and the final wavelength will be 6.28 Å. The simulations are focused around this wavelength range by restricting the wavelengths to 5 – 7 Å. For the simulations we used the McStas package [9]. The main components utilized were the guide and the guide\_curved components with the standard reflectivity profile, using \(\alpha = 5.07\) for the linear decrease in reflectivity beyond \(m = 1\). This corresponds to a reflectivity of 70% for the \(m = 4\) edge. We optimized the integrated intensity at the sample position which was defined as a rectangle of 2 cm \(\times\) 3 cm and a square of 1 cm\(^2\). The larger one is a standard size for quasielastic scattering experiments and the latter one resembles typical single crystal sizes or small amount biological samples. FIRES will be a high energy resolution instrument therefore larger divergence will be accepted to raise the intensity. Divergence was monitored to achieve a reasonably homogenous distribution. An inhomogenous divergence may influence the lineshape, in particular for single crystal experiments. We concentrated on curved guide designs to avoid direct line of sight. A direct line of sight will permit the transmission of high energetic neutrons from the proton pulse hitting the target and could create background peaks. The curvature radius was chosen to be \(R = 5000\) m. This radius of curvature corresponds to a characteristic wavelength of \(\lambda \approx 2\pi \sqrt{2a/R/k_\perp} = 1.9\) Å with \(k_\perp = 2.14 \times 10^{-2}\) Å\(^{-1}\) the maximum vertical wavevector for a \(m = 2\) guide and a guide width of \(a = 10\) cm. This large radius will allow to access large energy transfers with the silicon (111) reflection and the efficient use of the silicon (333) reflection.

3. Results
As a reference we took a guide similar to the existing one for the IRIS spectrometer [10], but now 90 m long. The resulting integrated intensity over the two sample sizes served as references and gain factors are quoted with respect to those intensities. The IRIS guide is a curved \(m = 1\) guide with dimensions 4.3 cm \(\times\) 6.5 cm, which is focused to end dimensions of 2.2 cm \(\times\) 3.3 cm.
by a 1.76 m long \( m = 2 \) linear focusing section.

As a first configuration we investigated a ballistic type of guide. The principle of such a guide is to widen the beam so that the number of reflections is reduced. A proper defocusing section will reduce the divergence according to the Liouville theorem and therefore the reflection losses. To obtain an optimized design, an iterative procedure was adopted. At first, the width and height of the ballistic section was varied, then the length and coating of the focusing section. The vertical and the horizontal lengths have been constrained to the same focusing length. After a further iteration now including the length and coating of the diverging part, an optimized set-up was found. The parameters for this set-up are indicated in fig. 1. The optimized value for the ballistic guide width is about a factor 4 larger than the width of the intensity distribution at the sample position, which corresponds to the achieved increase in accepted divergence with the \( m = 4 \) supermirrors in the focusing section. The gain factor is 2.3. The full widths at half maximum (FWHM) of the intensity distribution at the sample position are 2.4 cm horizontally and 3.3 cm vertically. The corresponding intensity distribution from a psd is depicted in fig. 2. A change of the coating in the long curved section to \( m = 3 \) did not provide a higher transmission, even by using larger m-values in the focusing and defocusing section. The next configuration studied was a combination of a curved guide with a nonlinear focusing section, an elliptic one. The component \texttt{guide\_tapering} from the McStas-package allows elliptic and other designs, but is restrictive in some options. The two focal lengths have to be provided and with the entrance dimensions of the guide, the ellipse geometry is fully determined. We created an elliptic shaped guide by calculating all guide segments individually using a Fortran program. For the elliptic focusing section at the end of the curved guide we added an ellipse which starts with the end dimensions of the optimized curved guide 9.8 cm \( \times \) 13.0 cm. These values are the minor axes of the ellipses in this case. The second focal point of the ellipse is fixed to the sample position, 0.35 m from the end of the guide. The major axis was then obtained by varying its length, for which we finally chose 8 m. Due to the high eccentricity of the ellipse the length of the segments can be chosen according to an exponential distribution \cite{11}, with longer segments at the center of the ellipse. For this focusing section we utilized 50 linearly tapered guide segments which resulted in a smallest length of 4.5 cm at the end of the ellipse. The coating was optimized to a distribution of m-values starting from \( m = 3 \) to \( m = 5 \) for the last 3 pieces. The guide-end dimensions are 2.2 cm \( \times \) 3.3 cm and the FWHMs of the intensity distributions are 2.4 cm \( \times \) 2.5 cm, resembling a more circular spot. The optimized design delivered a gain factor of 3.9 for the larger sample area and 4.0 for the smaller one, a factor 2 improvement over the ballistic design. Due to the guide curvature the horizontal divergence distribution is not symmetric as shown in fig. 3, but still more homogenous compared to the straight focusing guide.

The next natural step is to investigate a vertical elliptical guide over the whole length from

**Figure 2.** The intensity distribution at the sample position is shown for the ballistic guide set-up.

**Figure 3.** The horizontal (A) and vertical divergences (B) are depicted for the set-up with the elliptic focusing section. Due to the curvature of the guide the horizontal distribution is asymmetric.
Figure 4. Gain factors are depicted for the different configurations in respect to the IRIS-type instrument. Configuration 1 denotes the IRIS-type instrument, 2 the OSIRIS-type instrument, 3 the m2 ballistic guide, 4 the m3 ballistic guide, 5 the m2 curved guide combined with an elliptically focusing section, 6 the m3 curved guide combined with an elliptically focusing section, 7 the full elliptic geometry in the vertical direction and 8 the height restricted nonsymmetric bi-elliptic geometry.

the biological shield combined with a curved guide in the horizontal dimension. The horizontal guide geometry used the ballistic curved guide combined with the elliptic focusing section. This design resulted in a maximum guide height of 32 cm, but only negligible gains in intensity, which might be related to a too long distance between the focal point and the source and therefore an under illumination of the elliptic guide. Interestingly, a design which restricted the guide height to 10 cm and comprised of a combination of two elliptical sections delivered similar gain factors (configuration 8). The elliptical sections are not symmetrical, but are divided up in a quite long first one (70 m) and then a shorter second part. The partial illumination of the symmetric ellipse might explain the similar performance of this bi-elliptical set-up with reduced heights. Fig. 4 depicts a comparison of all of the obtained gain factors. It shows a two-step increase first by the ballistic guide geometry and second by the elliptic focusing designs. The clear increase for the elliptic designs combined with the more homogenous divergence distributions demonstrates a distinct advantage of these nonlinear geometries. Finally, we used the full elliptic guide component to get an idea what can be gained by a new guide design starting from the moderator and modifying the biological shield insert. This full elliptic design yielded ellipses with minor axes of 24.6 cm and 30.5 cm. The entrance dimensions are 1.6 cm × 2.8 cm and the guide end dimensions are 3.0 cm × 3.7 cm. With a \( m = 3 \) coating we got a gain factor of 12. This large gain factor might be understood due to a much reduced distance between the focal point of the ellipse and the moderator. For the used 6 Å neutrons the acceptance angle towards the source is a factor two larger with the full elliptic design compared to the \( m = 3 \) in-pile part. This factor 2 in one dimension might explain the overall factor 3 increase in gain with the full elliptic design.
4. Conclusions
From these results we conclude that a new guide design must consider also a change of the biological shield insert geometry. Even so larger gain factors for the curved design with modified inserts can be expected, we suppose that none will reach the high gain factor of the full elliptic design.

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