High Intensity Neutron Beams for Small Samples

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Abstract. As novel materials of excellent homogeneity can often only be grown in small quantities it is important to optimize the transport of neutrons from the moderator to the sample while keeping the background low. Using elliptically or parabolically tapered guides the losses can be strongly reduced such that 50% - 90% of the useful neutrons arrive at the sample. If not properly designed, however, the divergence at the sample becomes inhomogeneous. In contrast, pairs of nested Kirkpatrick-Baez mirrors in Montel geometry yield well focused beams with a compact phase space. The mirrors extract only the useful neutrons from the moderator and effectively interrupt the line of sight leading to a very low background. As the focal distances are typically several meters, the extraction of the neutrons and the installation of bulky sample environment is facilitated.

1. Introduction

An increasing number of metal and oxide samples for investigating effects of strong correlations are grown by optical float zoning. The resulting high quality single crystals have typically a volume of 1 cm^3. If investigated under extreme conditions the sample size shrinks further to a few 0.01 mm^3 - 1 mm^3 [1]. In the field of macromolecular crystallography and in biophysics the sample volumes are very small too. Therefore, one of the recent trends in neutron scattering is directed towards optimizing beam lines for the investigation of small samples. Indeed, the recent years have witnessed a rapid development of simple devices to focus neutron beams to small areas [2] and to transport neutrons with a high efficiency [3].

With the invention of neutron guides by Maier-Leibnitz [4] it became possible to transport neutrons over large distances by Ni-coated guide tubes. However, due to the small critical angle of total reflection given by $\theta(^0) = 0.099 m\lambda(\text{Å})$ where $m = 1$ for Ni, the transport was only efficient for cold neutrons. Using supermirror coatings [5], the index m can be increased up to $m = 7$ [6] thus allowing to even transport epithermal neutrons with reasonable divergence to instruments at spallation sources.

To reduce the reflection losses inherent to straight guides, truly curved elliptic guides [7] were proposed thus reducing the number of reflections of neutrons to approximately 2 while keeping the phase space of the neutrons compact [8]. For HRPD at ISIS, a gain of up to two orders of magnitude was reported [9]. There is no doubt that elliptic guides will improve the performance of instruments at spallation sources where each guide can be individually optimized. Klenø et al. [10] have shown recently that approximately 50% to 90% of the brilliance of cold and thermal neutron beams can be transported from the moderator to the sample using parabolic or elliptic guide geometries. Instruments at existing straight neutron guides can be improved by adding focusing guides at the down stream ends.

It is instructive to estimate the maximum possible intensity I at the sample position to judge the performance of a beam line. Assuming a loss free transport of neutrons from the moderator having a brilliance Ψ to the sample the intensity is given by

$$I = A \cdot \Delta\lambda \cdot \Omega \cdot \Psi. \tag{1}$$

Here, A, $\Delta\lambda$ and Ω designate beam size, wavelength band, and solid angle at the sample position, respectively. As an example, we consider the thermal beam port H12 at the ILL. Its brilliance at $\lambda = 1.2$ Å is $\Psi = 8 \cdot 10^{13}$ cm^{-2}s^{-1}Å^{-1}sterad^{-1} [11]. Assuming $\Delta\lambda/\lambda = 1\%$ and a horizontal and vertical divergence of 1^0 and 4^0, respectively, we end up with $1.2 \cdot 10^7$ neutrons per second hitting a sample with an area $A = 1$ mm^2. This procedure of estimating the intensity is very useful to benchmark the smallest sample size for which an experiment is feasible. Due to the theorem of Liouville there is no way to improve I further using passive means of focusing. If the beam line is designed and built properly, the quoted intensity can be approached within a factor of $\simeq 2$ using state of the art neutron optics while keeping the background at a low level.

In the following we discuss some basic principles on the adaption of neutron beams and the transport and focusing of neutrons. We will use simple concepts mostly based on parabolic and elliptic neutron optics. We do not show any Monte-Carlo simulations. Of course for the final optimization of a beam line numerical techniques are mandatory [12] but will not be discussed here. Due to the restriction in length not all details can be completely worked out in depth.

2. Adaption of Neutron Beams to the Sample

Often, beam lines are arranged along powerful guides, which extract as many neutrons as possible from the moderator. Beam size and divergence are defined close to the sample by means of collimators and slits. Thus, extensive shielding close to the guide and the sample is required to reduce the background to acceptable levels. A more efficient way of designing an instrument is to define the required phase space of the neutrons (beam size, divergence, bandwidth, time structure) as close as possible to the moderator and to extract only the neutrons to be used.

For the time being we neglect effects of bandwidth and time structure of the beam. Then, according to the theorem of Liouville, the phase space density $B = A\Omega$ is a constant. Let us consider a loss-less neutron guide 6 cm $\times$ 15 cm transporting neutrons with a divergence of 1^0. Within the guide, $B_{guide} = 90$ (cm ^{0})^2. Assuming a sample area of 1×1 cm^2 and an accepted divergence of 2^0, $B_{sample} = 4$ (cm ^{0})^2. Therefore, only $\simeq 4.0\%$ of the neutrons may be useful for the experiment while 96% have to be absorbed. In addition, the selection of the bandwidth for spectrometers reduces the intensity by another factor of 100, i.e. only $\simeq 4 \cdot 10^{-4}$ of the neutrons are actually being used requiring expensive shielding.

Concluding, the efficiency of a beam line can be strongly improved if only neutrons with the required phase space are extracted from the moderator. To reduce the contribution of fast neutrons and γ radiation it is best to extract the neutrons from a small area of the moderator. If this is not possible, a beam defining slit should be placed as close as possible to the moderator.

3. Elliptic Neutron Guides

Following the ideas of the last paragraph, neutrons are ideally extracted from an area of the moderator that has a similar size as the sample and the required divergence. Neglecting gravitational effects, it is the reflection by an ellipse that performs the required point to point transport of the neutrons (Fig. 1). As shown by Schanzer et al. [7], elliptic guides yield a reasonably homogenous beam at the sample position. Most neutrons are reflected while the contribution of the non-reflected neutrons (if there is no beam stop) is very small leading to an inhomogeneous divergence ψ at the sample. There will be a dip in intensity for angles $\psi < W/L$, where W is the width of the entrance and L is the length of the guide. For example, for $L = 40$

m and $W = 40$ mm, the dip is 10^{-3} rad (0.06^0) wide, i.e. small compared to the divergence of the neutrons. In two dimensions 4 peaks develop in the divergence distribution [13, 14].

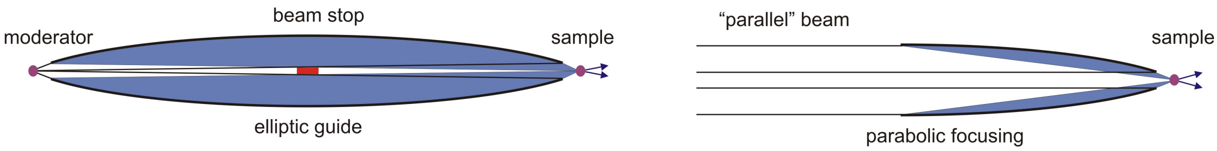

Figure 1. The transport of neutrons using an elliptic guide provides a point to point imaging of neutrons from the moderator to the sample. As the ellipse is not complete the divergence exhibits two peaks. The direct beam may be blocked by a beam stop. Parabolic focusing using a short neutron guide leads to a well-defined beam spot. However, due to the short length the divergence may become very inhomogeneous.

For an optimum design of elliptic guides, coma aberrations and halo effects should be considered [14]. Their importance scales with D/L where D is the spot size. Surprisingly, the waviness η has only rarely been taken into account although it is of similar importance. For example, $\eta = 1.0 \cdot 10^{-4}$ rad leads for a point-like object to a blurring of 1 cm for $L = 100$ m. Gravitation will further deteriorate the beam scaling with L^2. If properly considered one may use gravitation to interrupt the line of sight [15]. The experience from operating beam lines with elliptic guides, the mentioned deteriorating effects seem to be a minor issue [9].

Finally, let us make some practical remarks concerning the implementation of elliptic guides. Simulations for shielding demonstrate that the signal to noise for elliptic guides may be better than for curved guides [8]. Although, the beam stop (Fig. 1) interrupts the direct line of sight, the background at the sample position is still significant. The reason is that the guide sections close to the sample are directly illuminated by radiation from the moderator (Fig. 2) [16]. A simple remedy is dividing a single guide in two guides. Using an even number of guides has the further advantage that effects of halo, coma aberration [17], gravitation etc. are minimized.

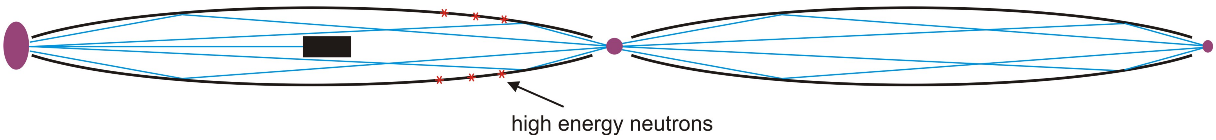

Figure 2. Guide sections close to the sample are directly illuminated by radiation from the moderatore (red stars) leading to a significant background. Dividing the guide into two sections improves the homogeneity of the beam and reduces the fast neutron background.

4. Focusing of Neutrons

Traditionally, neutron beams for small samples are configured by collimators and beam defining apertures leading to large losses in intensity and non-uniform illumination of the sample. If the last slit cannot be placed very close to the sample, the sample environment will be illuminated too leading to unwanted background. A large improvement can be made by installing truly curved elliptic or parabolic guides for focusing the neutron beam on the sample yielding gains of 25 and more [18].

Fig. 3 shows beam profiles of a focusing guide at the exit, focal position, and 200 mm away from the exit of the guide. The length of the guide is 500 mm and the exit size is 4×8 mm^2. The sides are coated with supermirror $m = 3$. The data was measured at the beam line CONRAD at HZB using neutrons with a wavelength of 3 Å and a CCD-camera [18]. Four beams evolve at the edges leading to one single spot at the sample position. Clearly, the divergence will be inhomogeneous showing four peaks by reasons explained in Fig. 1. A pronounced inhomogeneity is intrinsic to short focusing guides and becomes even more pronounced when the divergence of the incident beam is reduced as it leads to sharper peaks. Indeed, the width of the spot can be decreased to $\simeq 0.3$ mm if the divergence of the incident beam is reduced to 10'.

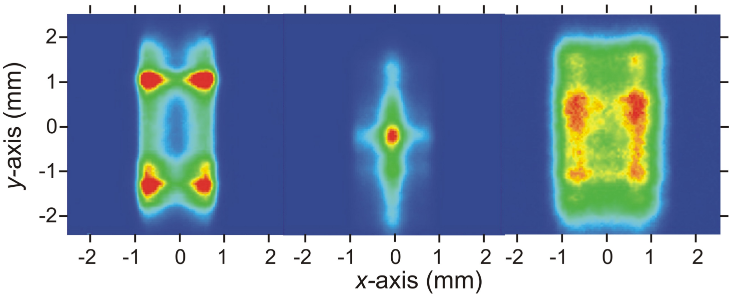

Figure 3. At the exit of the focusing guide, the neutrons leave the guide along the edges leading to a single sharp peak at the focal position $d = 80$ mm. Further away, the beam splits again into 4 beams.

To prove the usefulness of focusing neutrons with short flight tubes we have conducted diffraction experiments using the spectrometer PANDA at FRM II. Before the sample, the focusing guide from Fig. 3 was installed. Fig. 4(a) shows that the antiferromagnetic peaks in NiS_2 can be nicely resolved using a single crystal with the dimensions $1 \times 1 \times 0.1$ mm^3 [19]. Such small crystals fit into Bridgman cells for pressures up to 10 GPa. Fig. 4(c) shows inelastic data as measured at the thermal triple axis spectrometer PUMA using quartz with a volume of 0.75 mm^3. Although the signal is weak, the transverse acoustic phonon can clearly be resolved. More data on inelastic neutron scattering from small samples is reported in Ref. [20]. By adding a second (de)focusing guide after the sample the intensity can be further increased.

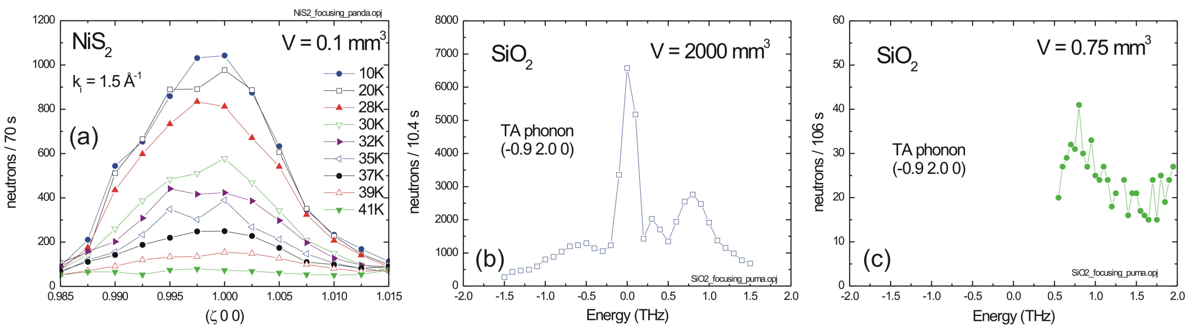

Figure 4. (a) Detection of magnetic order in NiS_2 using a focusing guide. The sample volume is only 0.1 mm^3. (b) Measurement of a transverse acoustic phonon in quartz from a sample with a volume $V = 2000$ mm^3. (c) Measurement using a focusing guide set-up with $V = 0.75$ mm^3.

5. Montel Optics

A major drawback of strong elliptic and parabolic focusing is the required small distance between the exit of the guide and the sample, $d \simeq 80$ mm, hindering the installation of bulky sample environment. A solution to this problem is the use of Montel optics [21, 22], where two elliptic (or parabolic) Kirkpatrick-Baez mirrors are arranged side by side. As shown in Fig. 3, the Montel geometry corresponds simply of using one beam emerging from one of the 4 corners of the guide leading to a focused beam with a well-defined divergence. The loss of a factor of 4 in intensity can be compensated for by doubling m from $m = 3$ to $m = 6$.

The major advantages of Montel optics are (Fig. 5): i) the beam size scales with the length L of the mirrors, ii) the distance $d \simeq L/2$ between the focal points and the mirrors is large, iii) the beam size can be tuned by an aperture at the first focal point, iv) the divergence can be adjusted by slits, and v) there is no direct line of sight between the two focal points. For an application for neutron reflectometry see Refs. [17, 23] and for a time-of-flight MIEZE spectrometer see Ref. [24]. Recently, design studies were conducted for the beam line SNAP, at SNS [25]. Using metallic substrates [26] it is anticipated that beam sizes of 30 μm or below can be obtained.

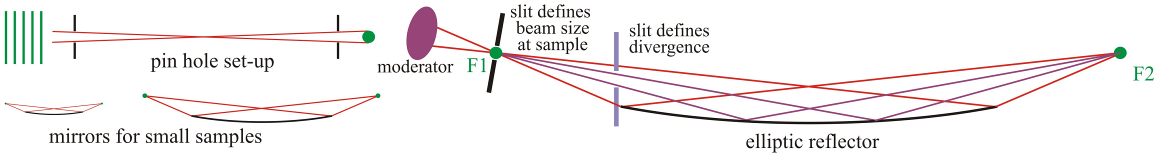

Figure 5. For a pin-hole set up [27] the beamsize is defined by means of slits close to the sample, which usually restrict the divergence leading to low intensity and high background. An elliptic mirror provides a point to point imaging. The beam size and the divergence can be adjusted by slits close to the moderator thus allowing to reduce the size and improve the performance of the moderator. Large (small) mirrors allow the illumination of large (small) samples.

Typically, a minimal guide system will consist of two or more Montel mirrors. An even number of elements is of advantage as coma aberrations, halos, and gravitational effects are reduced. In between the mirrors, beam defining elements such as choppers, apertures, monochromators, polarizers etc. can be inserted [24]. As typical lengths of Montel mirrors are of the order of 10 m - 20 m, the entrance of the first mirror can be placed approximately 5 m away from the moderator, i.e. in a regime of reduced radiation. This geometry allows a simple adaption of beam optics for new neutron scattering instruments as the optical parts are placed at the boundary of the biological shielding and can easily be modified. Moreover, as neutrons are extracted from a small spot of the moderator only, its size can be strongly reduced leading possibly to a higher brilliance. It is clear that the use of Montel optics for future beam lines will significantly improve the performance of neutron instrumentation due to the well-defined phase space and the extremely low background. Moreover, costs for shielding can be massively reduced.

6. Conclusions

Summarizing, we have shown that the significant technological advances in the development of supermirror coatings and the step from using straight guides via elliptic guides to Montel optics will lead to a significant improvement of neutron beam lines. Respecting the limits imposed by Liouville's theorem it is rather straightforward to design a beam line and predict its performance.

For beam lines requiring highest intensity such as inelastic chopper spectrometers, a combination of an even number of elliptic guides may be the optimum choice. For most other beam lines an even number of Montel mirrors may yield highest performance. This view is at variance with propositions of going away from a purely elliptic transport for neutrons [28]. Many beam lines built so far have proven that the elliptic approach is rather straightforward from the design point of view and that it works very well yielding the expected beam quality [9].

To guarantee the proper transport of the neutrons from the moderator to the sample, an active surveillance system to control the alignment of the neutron guides may be required. Such a system would also allow to actively adapt the complete guide system for the optimum transport of neutrons within a predefined wavelength band thus reducing gravitational effects. Sophisticated alignment techniques have been developed for the Compact Linear Collider CLIC at CERN, where transverse positions of components have to be aligned and stabilized to within 10 μm over distances of 200 m [29].

To take full advantage of all the possible neutron gains using advanced reflecting optics attention should also be paid to the development of radiation-hard chopper systems that can be placed as close as possible to the moderator to allow i) a precise chopping of the beam due to the small beam size [3] and ii) a reduction of frame overlap. Further, as the neutron yield from spallation sources and high flux reactors is limited intense research should be devoted to producing highly brilliant neutron beams using for example intense γ-rays from electron recovery linacs [30]. If such neutron sources can be realized, similar dramatic increases in brilliance will become feasible as realized with x-ray synchrotron sources.

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