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Nested neutron microfocusing optics on SNAP

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Abstract The high source intensity of the Spallation Neutron Source (SNS), together with efficient detectors and large detector solid angles, now makes possible neutron experiments with much smaller sample volumes than previously were practical. Nested Kirkpatrick–Baez supermirror optics provide a promising and efficient way to further decrease the useable neutron sample size by focusing polychromatic neutrons into microbeams. Because the optics are nondispersive, they are ideal for spallation sources and for polychromatic and wide bandpass experiments on reactor sources. Theoretical calculations indicate that nested mirrors can preserve source brilliance at the sample for small beams and for modest divergences that are appropriate for diffraction experiments. Although the flux intercepted by a sample can be similar with standard beam-guided approaches, the signal-to-background is much improved with small beams on small samples. Here we describe the design, calibration and performance of a nested neutron mirror pair for the Spallation Neutrons At Pressure (SNAP) beamline at the SNS. High-pressure neutron diffraction is but one example of a large class of neutron experiments that will benefit from spatially-resolved microdiffraction.

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1 Introduction

Neutron experiments are typically starved for neutrons and as a result, most neutron experiments require large samples (1–1000 mm^3) that can use large neutron beams. This restriction limits the samples that can be studied and makes it difficult to study heterogeneous samples or small samples in large environmental chambers. For example, the typical grain size for polycrystalline materials is on the order of 10^{-9} to 10^{-3} mm^3. The development of intense neutron sources like the SNS and the use of beam guides and efficient area detectors has decreased the required sample size, but the performance of traditional pin-hole-based neutron optics scales like the fourth power of the beam size for small beams [1]. As a result beam size can be reduced by less than a factor of 2 for an order of magnitude improvement in source brilliance (or detector efficiency). True focusing optics provide an alternative path toward small beams; beam intensity scales with the square of the focal spot size with focusing optics. Recently, Kirkpatrick–Baez optics have been demonstrated as an efficient method to achieve <100 μm spots [1–3]. For small beams, KB optics can nearly preserve source brilliance into the focused beam emittance (size x divergence). Based on earlier results, we estimate that beams as small as 15–25 μm can be used for single-crystal high-pressure research on the SNS. We have adopted this spot size as a goal for efficient neutron focusing optics.

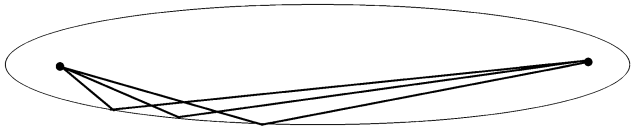

Fig. 1 An elliptical mirror focuses from one focus onto the other focus

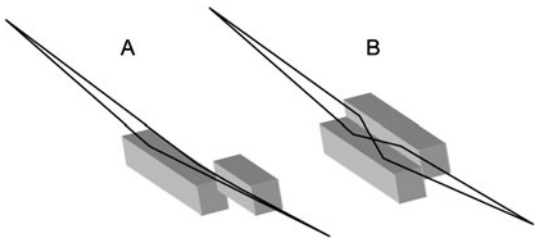

Fig. 2 (**A**) Standard Kirkpatrick–Baez sequential mirrors have orthogonal scattering planes and are arranged such that neutrons are deflected and focused first in one plane, and then in the orthogonal plane. All rays strike the primary mirror first and then the secondary mirror. (**B**) With "nested" KB mirrors, the two mirrors have the same object and image distances. Some rays strike one mirror and other rays strike the other mirror first. For a ray to strike both mirrors, it must intersect near the corner where the two mirrors come together (see for example Fig. 3)

The basic approach to imaging neutrons with a bent Kirkpatrick–Baez mirror is illustrated in Fig. 1, which shows the classical focusing of rays by specular reflection from an elliptical surface. In the scattering plane, an elliptical surface intercepts rays from one focus and converges them onto the other focus through specular (angle in = angle out) reflection. In the standard KB geometry, Fig. 2A, sequential focusing from primary and secondary mirrors at right angles is used to doubly focus a beam. By nesting the mirrors (Fig. 2B), the solid angle that can be collected into the focus is increased.

Although an elliptical surface satisfies the geometrical condition of specular reflection for all rays from one focus to the other focus, neutron mirror reflectivity is typically low except for glancing angles. For a natural Ni mirror, the reflectivity is low if $\sin\theta > \lambda(\text{nm})0.217(\text{nm}^{-1})/4\pi$; http://www.swissneutronics.ch/products/concept-supermirrors.html. Here λ is the neutron wavelength in nm, θ is the incident angle of the beam with respect to the mirror surface in radians and the momentum transfer constant 0.217 (nm^{-1}) is a physical property of Ni. With a neutron supermirror, the mirror reflects efficiently at angles M times larger than for natural Ni. Consequently, the condition for efficient reflection of neutrons is given by,

$$\sin\theta \sim \theta < \frac{\lambda(\text{nm})M}{57.9} \tag{1}$$

As seen in (1), large M numbers indicate larger angles and therefore allow for the collection of larger beams. Mirrors with $M \sim 3$ can be made with high reflectivity and mirrors with $M \sim 5$ are at the frontier of neutron optics. For thermal neutrons, $\lambda \sim 0.1$ nm, glancing angles are essential even for the largest M mirrors.

Because neutron optics operate far from the diffraction limit, and because the aberrations for Kirkpatrick–Baez ***demagnifying*** optics are small, microbeams are possible by satisfying two conditions: (1) the geometrical demagnification, m, of the object size, O, must be less than the required spot size, S ($mO < S$); and (2) the root-mean-square figure deviations from the design ellipse must be small. If we assume the figure errors have a Gaussian distribution, and that the mirror length is small compared to the image distance, then the blurring due to mirror figure errors can be estimated at,

$$S_{\text{Blur}} \sim 4\sigma'_{\text{RMS}}\sqrt{2\ln 2} = 4.7F_2\sigma'_{\text{RMS}}. \tag{2}$$

Here F_2 is the image distance, F_1 is the object distance, $m = F_2/F_1$ is the magnification, σ'_{RMS} is the root-mean-square slope errors of the figure and S_{Blur} is the full-width-at-half-maximum blur at the focus. A more accurate description of the estimated blur will take into account the both the slope errors and their position along the mirror.

The blur condition above complicates the design of ***bent*** mirror optics. For example as F_2 decreases, the blurring for a given figure error also decreases. However, as F_2 decreases, the local radius of curvature must shrink for a given glancing angle, θ. For example, the local radius for focusing with a KB mirror is given by,

$$R = \frac{2F_1F_2}{(F_1+F_2)\sin\theta} \sim \frac{2F_2}{\sin\theta}_{F_1 \gg F_2}. \tag{3}$$

Unfortunately thick easily polished mirrors are difficult to bend to a small radius, while thin mirrors are hard to make with small figure deviations from flat. Thin (bendable) mirrors are also more sensitive to gravitational sag and other contributions that compromise the ultimate ability to conform the mirror surface to a specific shape.

2 Experiment

2.1 Mirrors and focusing strategy

Based on an initial prototype KB mirror system, a new "nested" KB mirror system was designed with the horizontal and vertically deflecting mirrors nested against each other with equal image and object distances (Fig. 2B). The bending approach was based on the simple bending scheme pioneered by the Advanced Light Source, ALS [4], and used successfully on the sequential neutron KB prototype [1–3]. The complexity of a nested design was justified by the larger divergence that can be collected by this geometry and by the smaller F_2 of the mirror pair compared to the F_2 of the primary mirror in a sequential mirror system.

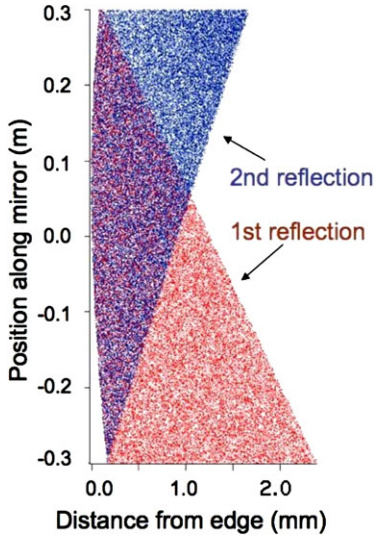

Fig. 3 Intercept of reflected rays along a nested mirror showing the displacement from the corner where the mirrors touch

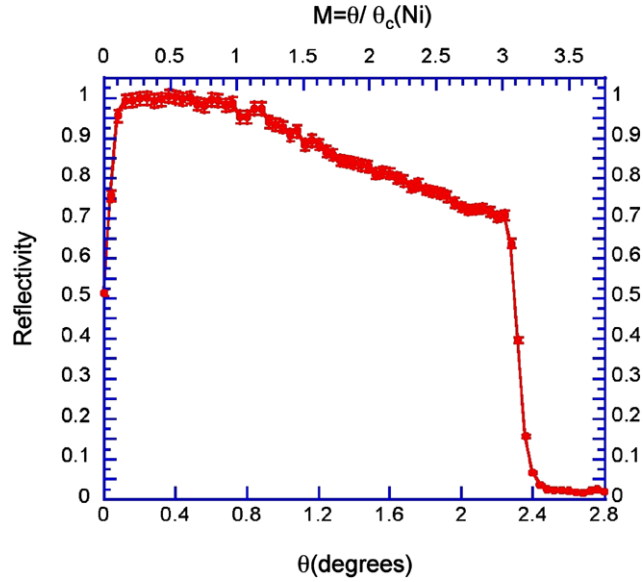

Fig. 4 Reflectivity of the supermirror, measured at $\lambda = 0.75$ nm

One tremendous complication of the nested geometry is the need for good surface figure at the edge of one of the mirrors. As shown in Fig. 2B, the mirrors are nested so the beam deflects from the edge of one mirror and from the middle of the other mirror. Figure 3 illustrates the ray-trace calculated intercepts along the mirrors for first and second reflections. As illustrated in Fig. 3, all of the mirror reflections occur near the corner where the two mirrors touch. Unfortunately, mirrors with good edges are atypical. For this experiment, special mirrors polished on all 4 sides were procured. These 0.6 m long mirrors have very good surface figure but are relatively thick for bent mirrors and are therefore very stiff.

2.2 Mirror coatings

The mirrors were coated with a neutron supermirror in order to increase the reflection angles and thereby increase the numerical aperture. As mentioned in the introduction, for a given wavelength range, larger M number mirrors reflect efficiently at larger angles and therefore make it possible to increase the focused neutron flux at the sample. $M = 3$ supermirrors were coated on both mirrors, by D.C. magnetron sputtering at the Institut Laue–Langevin (ILL). The coating consists of 560 layers, alternatively Ni(V) and Ti, with individual thicknesses ranging from 4.5 to 60 nm. Figure 4 shows the typical specular reflectivity measured on one of the mirrors after coating.

The measurement was done at the ILL as a function of incidence angle, for a monochromatic beam of 0.75 nm wavelength. It is worth emphasizing that the substrate microroughness strongly influences the supermirror reflectivity, as it usually replicates in successive interfaces. Since the KB mirror system focuses onto the sample using two reflections, the focused brightness scales as the square of the supermirror reflectivity. Thus the roughness has to be as low as possible, which puts an additional constraint on the polishing of the mirrors. In this case, the R.M.S. roughness values of the mirrors deduced from x-ray reflectivity measurements before coating were between 0.8 and 1.4 nm. The cut-off wavelength reflected by the focusing mirrors can be deduced with formula (1), replacing θ by the highest incidence angle given by the geometry.

2.3 Figure measurements/ Re-measurements

The available distance between an adjustable aperture that serves as the object and the sample position (image) on SNAP is ∼7 m. The mirror surface figure was measured and optimized with a specially designed long-trace-profiler, LTP, that could be oriented to measure either vertically or horizontally deflecting mirrors in the orientation in which they are used [5]. The mirrors were measured prior to installation on SNAP. This drastically reduces the degrees of freedom during alignment. The target goal was to achieve a nominal mirror angle, θ, of about 3.5–4 mrad, with an image distance of ∼0.5 m (0.2 m clearance). However, the simple bending mechanism became ineffective due to excessive tensile forces for $F_2(m)/\theta < 200$. The best compromise was found under the following bent mirror conditions (Table 1).

One point of interest is the stability of the bent mirrors. We note that the mirrors were measured before and after the SNAP experiments. After neutron measurements and a round trip of ∼6 miles between the LTP and the SNS, the remeasured mirrors were in good agreement with the original measurements (Table 1).

2.4 Focal spot size measurements on SNAP

The neutron mirror focusing system was installed on the SNAP beamline. The object was an adjustable aperture located ~6.17 m from the center of the two mirrors. A BN knife edge was positioned 0.83 m from the mirror center to measure the beam spot size. The mirror angles were set using the displacement of the reflected beam from the incident beam at the detector. Once the mirror angle was set, the mirror angle was adjusted to optimize the spot size. The full mirror length was used for focusing. The results for 3 object sizes are shown in Fig. 5. The beam was only briefly optimized for a 2 mm object size and at 0.5 mm object size the signal-to-noise was poor. The measurements at 1 mm object size however are roughly consistent with the predictions based on the LTP surface errors measured and on ray-tracing. We note that the RMS size of a uniformly illuminated 2 mm slit is 0.576 mm which yields a FWHM for a Gaussian of 187 which is in good agreement with the ray-tracing estimate.

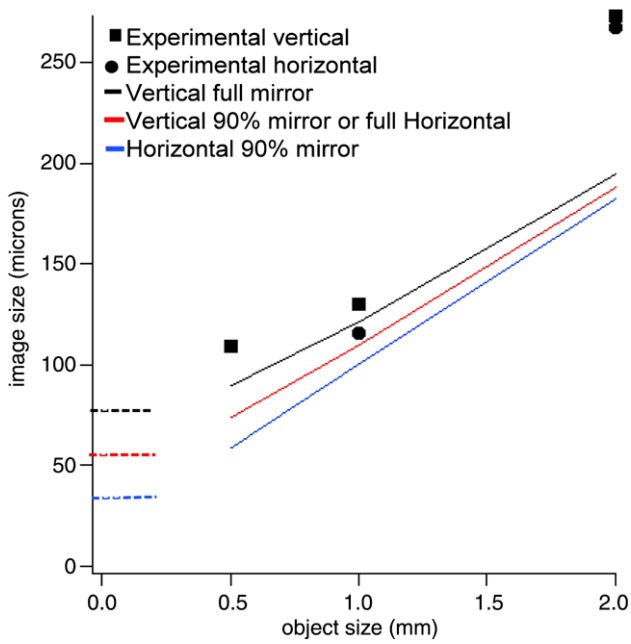

Fig. 5 Measured spot sizes on SNAP compared with the predictions based on ray-tracing optics and the measured figure

3 Discussion and future improvements

The ultimate beam size predicted from the mirror figure errors is given by the blur contribution (2) in the limit of a negligibly small source. The limit is indicated on Fig. 5 for the two mirrors and for various factions used of the mirror surface. As indicated in Fig. 5, the ultimate spot size using ~80% of the beam (90% × 90%) is estimated to be about 33 × 55 μm^2. This is more than a factor of 2 larger than our goal (15–25 μm). In addition, the large radius achievable with the bending mechanism, limited F_2/θ and limits the flux on the sample. Even if the mirrors were perfectly bent, their limited (0.6 m) length and long image distance ($F_2 = 0.83$ m) restricts the total flux at the sample by limiting the beam divergence. With the original goal of ~200 mm clearance ($F_2 = 0.5$ m) we estimate a gain of $0.5^2/0.83^2 \sim 2.7\times$ the flux as with the compromised radius.

We have therefore modified the bending geometry to apply nearly pure and independent bending moments to the

Table 1 Measured mirror parameters before and after testing on SNAP

	F_1 (m)	F_2 (m)	θ (mrad) before	θ (mrad) after	σ'_{RMS} 93% mirror before	σ'_{RMS} 93% mirror after
Vertical	6.17	0.83 m	3.74	3.45	20.5 μrad	16.6 μrad
Horizontal	6.17	0.83 m	3.87	3.89	9.6 μrad	6.6 μrad

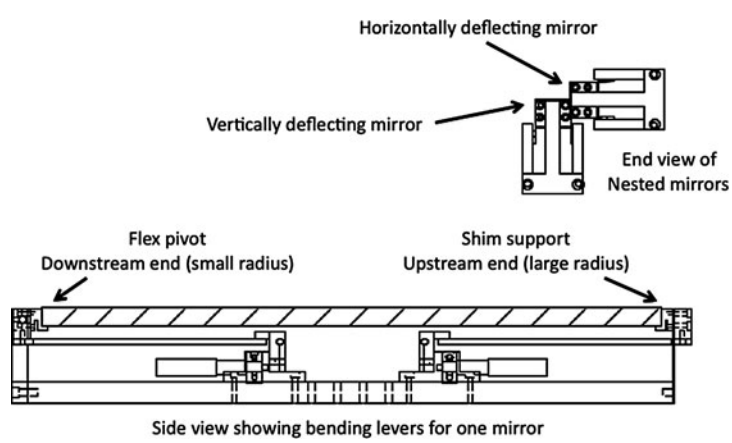

Fig. 6 New mirror bending mechanism designed to apply independent bending moments to the mirror ends

mirrors. The mirror bender design is shown in Fig. 6. This design is also discussed in Ref. [4], but is somewhat more complicated than the original leaf spring approach. In the new geometry the downstream end of the mirror is supported by a flex pivot that allows for rotations but limits translations. A lever attached to this end is pushed to apply a bending moment to the downstream end of the mirror. The upstream end of the mirror is supported by a stiff leaf spring. The leaf spring allows for small rotations and accommodates small displacements of the mirror. The new design will be calibrated on the LTP and then tested at SNAP. In principle, this design applies almost pure and independent bending moments to the mirrors and will not be limited by tensile loads. Based on our previous experience with the original bending approach, the original design is adequate for slightly thinner mirrors or for cases where the image distance is larger.

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