LA-UR-05-5874

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Intended for: ICANS-XVII
17th Meeting of the International Collaboration on Advanced Neutron Sources
April 25-29, 2005
Santa Fe, New Mexico

Los Alamos NATIONAL LABORATORY EST. 1943

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Kirkpatrick-Baez Super Mirror Optics For Intense Neutron Microbeams

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Abstract

High-performance neutron super mirrors in the Kirkpatrick-Baez (KB) geometry can efficiently focus polychromatic neutron beams to small spots. We have recently demonstrated near ideal performance with a prototype system designed to produce broad-bandpass neutron beams less than 100 μm in size with wavelengths between 0.8 and 1.4 Å . We describe the design criteria for the prototype system, and show that for thermal neutrons and typical beamline distances, optical aberrations and gravitational dispersion are negligible. We also describe ways to improve the performance of KB optics and techniques to extend the advantages of KB supermirror optics to long wavelength neutrons (4-6 Å) where gravitation dispersion is significant.

1. Introduction

Focusing of polychromatic neutron beams is essential for many experiments with small samples. In particular size-matched neutron beams allow for the best signal-to-noise, S/N, when a small sample is surrounded by an environmental chamber or other mounting hardware. Small beams are also essential for heterogeneous materials where properties change over a small length scale and *polychromatic* focusing is essential for spallation sources or for reactor experiments that can utilize a broad neutron spectrum.

Although many methods have been proposed and tried for focusing neutron beams to small dimensions[1-3], most are either inefficient or poorly matched to wide-bandpass beams. Other methods can increase neutron flux for modest sized beams, but are difficult to extend to beam sizes below one millimeter.[4] As part of an effort to optimize neutron micro Laue diffraction experiments, ray-tracing calculations have been used to study the focusing and brilliance preserving properties of various optical schemes. These calculations indicate that for most reasonable geometries, Kirkpatrick-Baez (KB) mirrors[5] can nearly preserve source brilliance[6] (neutrons/s/mm^2/mrad^2/Δλ) while producing polychromatic micron-sized neutron beams.

Although the KB mirror systems have a divergence limit somewhat lower than is typical for beam guided beams, the divergence within a *small* beam is greater than required by typical neutron optics to achieve 100 μm sized beams[6]. As a result, for small samples, huge improvements in performance are possible compared to traditional neutron optics. As described in reference 6, supermirror based KB optics are generally preferred to beam-guide systems when the ratio of the sample size, S, to the sample distance, D, (distance from last optical element to sample) is less than ~0.007; S/D <0.007. This ratio is reached in many situations, but there are additional technical complications due to the difficulty of manufacturing large KB mirror systems that make the advantages of KB mirrors most pronounced for small beams.

As described below and in reference 7, more complicated mirror focusing systems can extend the advantages of KB mirror optics to large beams, especially for cases where very large divergences are acceptable. However for many diffraction experiments, simple KB optics represent a good compromise of reasonable divergence, ease of fabrication and high performance.

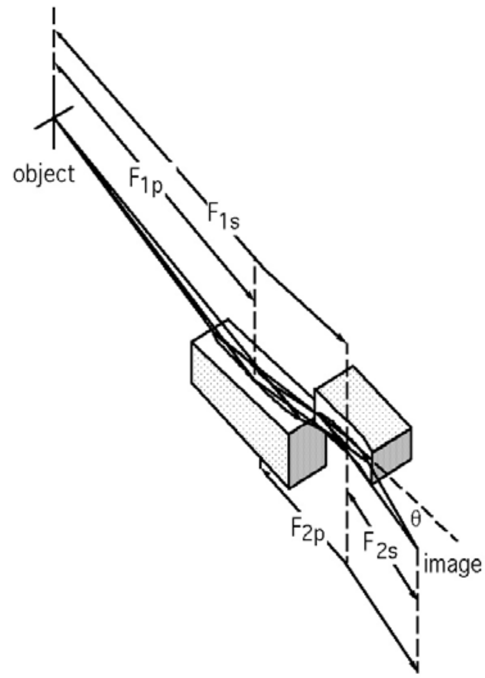

Figure 1: Schematic of a Kirkpatrick-Baez mirror pair. Each elliptical mirror focuses nearly independently in their orthogonal planes of scattering. The object lengths F_{1P} and F_{1S} are designated for the primary (first) and secondary (second) mirrors of the pair. The image distances are designated F_{2P} and F_{2S}. The doubly focused image is produced at a distance $F_{1P}+F_{2P}=F_{1S}+F_{2S}$ from the object.

2. Design rules for neutron KB mirror systems

The Kirkpatrick-Baez (KB) geometry (Fig. 1) uses crossed elliptical mirrors in grazing incidence to condense neutron beams. The mirrors focus independently in orthogonal planes of scattering with object distances F_{1P} and F_{1S} and image distances F_{2P} and F_{2S}. At a given scattering angle, θ, neutron supermirrors efficiently reflect neutrons with wavelengths greater than a critical value, λ_c, that scales linearly with the reflection angle,

$$\lambda > \lambda_c(nm) \sim 56.5\frac{\theta(rad)}{M}. \tag{2.1}$$

Here M refers to the ratio of the supermirror critical angle compared to the critical angle of a nickel neutron mirror. For λ_c=0.1 nm, the critical angle for an M=3 mirrors is ~5.3 milliradian (0.3°). Alternatively, for a given wavelength, λ, a supermirror efficiently reflects at angles below a critical angle;

$$\theta(rad) < \theta_c \sim \frac{M\lambda(nm)}{56.5}. \tag{2.2}$$

Because neutron supermirrors reflect neutrons specularly, ($\theta_{In} = \theta_{Out}$), they are inherently nondispersive; all wavelengths greater than λ_c are focused nearly equally.

The absolute maximum divergence that can be collected by a supermirror focusing in the plane of scatter is $2\theta_c$. In a practical mirror, with mirror length approximately equal to the focal length, a divergence of about θ_c is condensed onto the sample. Because the mirrors in a KB mirror system are sequential, a typical arrangement (Fig. 2) has a primary mirror with an image distance, F_{2P}, equal to its mirror length. The secondary mirror has an image distance and mirror length $F_{2S}=F_{2P}/3$. The free distance between the last mirror and the sample is therefore $F_{2P}/6$ (see Fig. 2). With this arrangement both mirrors collect a divergence of about θ_C onto the sample. If for example it is desirable to reduce the divergence in one axis while increasing it in the orthogonal axis, then the mirror lengths can be slightly adjusted.

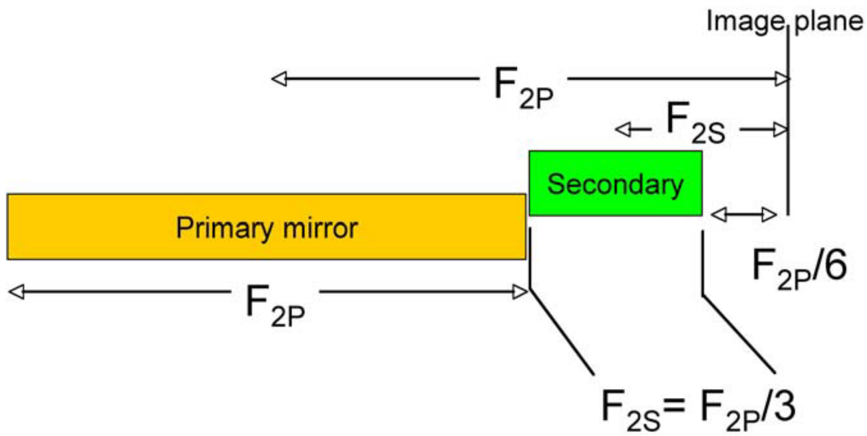

Figure 2: Schematic of a Kirkpatrick-Baez mirror pair showing how they can be arranged to collect equal divergence onto the sample. The clearance between the last mirror edge and the sample depends on the size of the mirrors.

In general because KB mirrors are focusing devices, more free space between the end of the last mirror can be purchased at the expense of larger and more expensive mirrors and a smaller object. As shown in Fig. 3, a mirror with the same ratio of image distance to mirror length collects the same divergence onto the sample, and for perfect mirrors has nearly identical performance. Figure errors in the mirror surface however, blur the image according to,

$$S_b \sim 4.7\sigma' F_2. \qquad (2.3)$$

Here S_b is the FWHM of the blurring from a mirror surface due to an approximately Gaussian distribution of slope errors with root-mean-square σ' and with an object distance F_2. Clearly as F_2 increases, blurring due to slope errors increases and the size of the mirror increases. Because large mirrors with good slope errors are expensive, it is cost effective to use small mirrors whenever possible. Of course many applications have a minimum clearance requirement that sets the focal and mirror lengths.

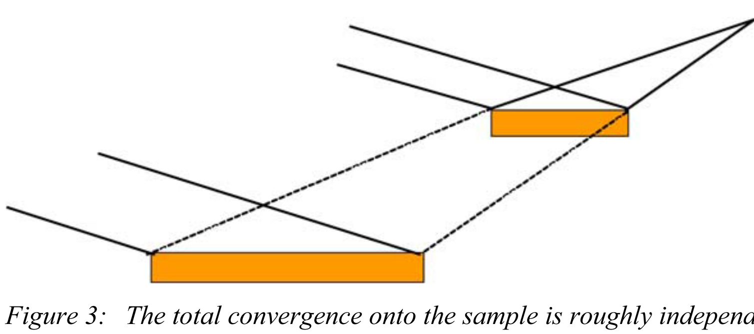

Figure 3: The total convergence onto the sample is roughly independent of the distance from the sample to the mirrors as long as the ratio of sample distance to mirror length remains constant. However, long distances (large mirrors) allow for more clearance between the mirror and the sample while short distances (small mirrors) reduce costs and complexity of mirror fabrication.

2.1 Prototype design.

To demonstrate the feasibility of nondispersive neutron focusing with KB supermirrors we have designed and built a simple KB mirror system based on bent mirrors. First experiments with the prototype have been reported previously.[6] The prototype system is designed to have a flexible sample distance of about 0.1 to 0.15 m with a targeted focal spot size of less than 100 μm and a critical wavelength of around 0.8 Å. The primary (horizontally focusing) mirror is 0.6 m long and the secondary (vertically focusing) mirror is 0.2 m long. The M~3 supermirrors have a reflectivity of about 70% and a critical angle of about 4.2 mrad for 0.08 nm neutrons. Back-of-the-envelope calculations indicate that gravitational dispersion should be small for $\lambda<2$ Å and for the object/image distances used. The choice of a small vertically-focusing mirror as the secondary mirror further reduces distortions of the mirror surface due to gravitational sag, and reduces the effect of gravitational dispersion in the vertical plane. We discuss gravitational dispersion in more detail later with respect to performance at 4-6 Å.

3. Performance of prototype KB optics

First measurements[5] were made on LANSCE flight path 5 (FP5). The object for the focusing system was formed by an adjustable BN slit set to a size of 1 mm horizontal by 3 mm vertical. The geometrical demagnification was approximately 6:1 in the horizontal and 17:1 in the vertical. The estimated full-width at half maximum, FWHM, image size with ideal focusing was therefore 101 μm horizontal x 107 μm vertical assuming the root-mean-square, RMS, size propagated as a Gaussian from the rectangular slit. The simple demagnified slit size was 166 x 174 μm^2. The measured FWHM of the image was about 185 μm horizontal at 1, 1.2 and 1.5 Å. The measured FWHM of the vertical image was 145 μm at 1 Å ;108 μm at 1.2 Å; and 64 μm at 1.5 Å. The large variation in the vertical spot size as a function of wavelength appears to be primarily due to uncertainties introduced by the large knife edge step size used for the vertical measurement (100 μm) compared to the step size used for the horizontal measurements (50 μm). Nevertheless, the focal spot positions agreed for all wavelengths in both vertical and horizontal directions to a few microns. For the FP5 measurements the optics were pre-aligned using a laser and only a few iterations of the focusing conditions were attempted. The estimated gain was about 37.

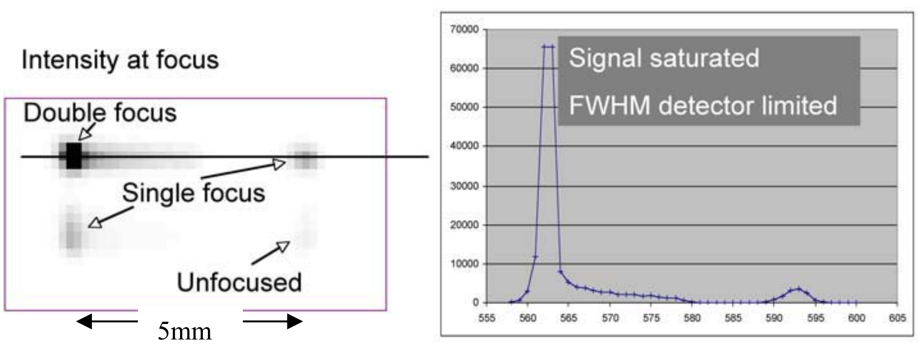

Figure 4: The beam intensity was measured at the focal plane using a neutron sensitive image plate. The 2D beam intensity distribution is illustrated on the left with four regions of intensity characteristic of a KB mirror system: "gang of four". The weak beam on the lower right is due to neutrons that pass over or through both mirrors. The weak beam on the upper right is due to neutrons that are deflected only by the vertical focusing mirror. The weak beam on the lower left is from neutrons deflected by the horizontal focusing mirror. The intense spot in the upper left corner is the doubly focused beam. We note that the undeflected and singly deflected beams can be removed. A line scan through the 2D image shows that the signal is saturated at the doubly focused position. Because the resolution of the image plate is insufficient to accurately determine the gain of the system, knife edge scans in front of a He_3 detector were used.

Further tests were carried out on beamline L3 at Chalk River.[7] At Chalk River the object was formed by a 1x3 mm slit set in front of a small side-deflecting mirror that replaced the monochromator crystal of the beamline. The deflected beam was focused by the KB optics onto a real-time area detector that allowed for rapid adjustment of the positions and angles of the two mirrors. The geometrical demagnification at L3 was about 7:1 horizontal by 22:1 vertical. The theoretical demagnified image size was therefore about 87 μm horizontal by 83 μm vertical assuming the FWHM propagated as a Gaussian from the rectangular slit. The measured spot size was 89 x 90 μm^2 with an estimated gain[7] of more than 100.

4. Beyond prototype optics

4.1 Ways to increase divergence and increase efficiency for larger beams

Although the prototype worked nearly ideally, there are significant improvements that can be introduced into new devices to improve performance and extend the useful range of applications. For example, as described above, KB mirrors preserve source brilliance within a *restricted* emittance that is typically smaller than can be passed by neutron beam guides *for large samples*. We propose two methods to extend KB technology to increase the emittance. In one method (Fig. 5a) mirrors are nested against each other so that some rays are first reflected upward and some first reflected sideways. This approach increases the divergence that can be collected from about θ_c to about 1.6 θ_c. As this increased divergence is in both directions the total flux density can be increased by about a factor of 2.5. This kind of KB mirror system is already in use for compact x-ray focusing systems.

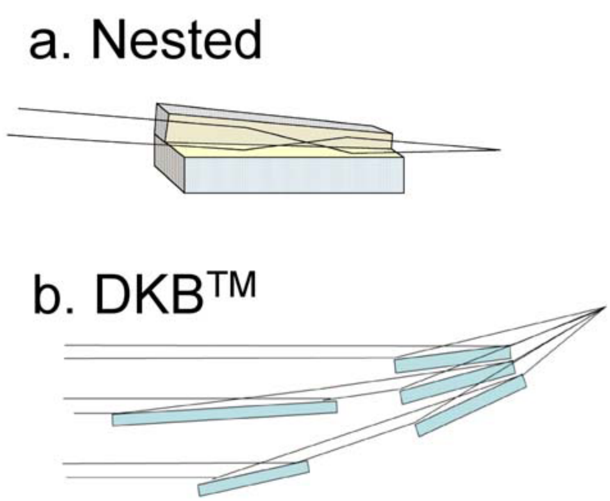

Figure 5: (a) With nested mirrors both mirrors act as the primary and secondary mirrors with some rays hitting one mirror first and some rays hitting the other mirror first. Both mirrors can be longer than a primary mirror in a standard KB mirror system with the same clearance and can simultaneously can have a shorter image distance. As a consequence more than twice the incident beam can be focused onto the sample. (b) Deflected KB optics are made up of flat mirrors and identical elliptical mirrors. Up to 5 times more beam than a conventional KB mirror system can be collected in each axis for a total flux gain of 25 over conventional KB mirror systems. This provides a theoretical gain compared to a slitted beam of ~2500 for a 100 μm spot and 100 mm clearance between the last optical element and the sample.

A second more radical approach uses additional mirrors to deflect parts of the incident beam. A one-dimensional schematic of this approach (with a gain of 3) is shown in Fig. 5b. Some rays reflect off only a single elliptical focusing mirror (mirror 1) and are focused on the sample. Other rays reflect first off a plane mirror (at ~$\theta_c/2$) (mirror 2) and then off a second elliptical mirror with the same figure as mirror1. These rays also focus on the sample, but with the average incident beam angle displaced by θ_c. Other rays can be deflected first by a single mirror at θ_c, or by a series of plane mirrors. This approach has the potential to extend mirror collection angles to collect very large divergences.

4.2 Application to longer wavelengths

At long wavelengths, gravitational dispersion becomes a serious consideration for simple KB optics. Copley[8] explored this effect with ellipsoidal mirrors for very long wavelengths (10-30 Å) and flight paths (~10 m). He studied a partial remedy by adjusting the source position (as a function of wavelength) to compensate for the fall of the neutron along the object distance. Even this approach however was only partially able to compensate for the observed dispersion and aberrations.

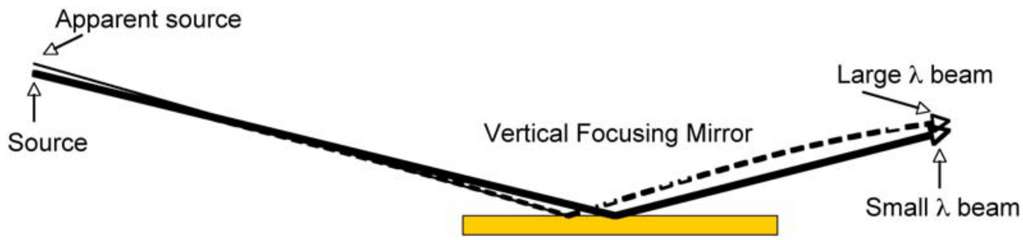

Figure 6: Gravitation dispersion effect on a slow neutron beam. The beam falls both before and after reflecting from the mirror. The angle of reflection from the mirror also changes due to the change in direction of the neutron beam. Reversing the mirror from an up to a down deflection does not change the magnitude of the gravitational dispersion.

From a focusing perspective there are two important consequences of gravity as the beam approaches a vertically focusing KB mirror: (1) the beam falls which changes the apparent vertical source position and mirror intercept, and (2) the neutron beam velocity vector changes direction which changes the angle of incidence on the mirror and also changes the apparent source position. These two- partially compensating-effects are shown schematically in Fig. 6.

Because a neutron source typically has divergence sufficient to completely cover the length of a KB mirror surface (even with small gravitational displacements) the most important effect is the displacement of the apparent source position. The apparent source displacements due to actual beam displacement and due to changes in beam direction both scale linearly with the acceleration of gravity and linearly with the square of the time from the source to the mirror. We assume the small displacement limit where the change in beam direction has a factor of two larger influence on source position than gravitation fall and has an opposite sign. We also assume that the mirror scattering angle is small, and that the incident beam is approximately parallel to the earths surface. With these assumptions, and substituting in the velocity of neutrons, v(m/sec)=3958/λ(Å) it is straightforward to estimate the apparent source displacement of long wavelength neutrons compared to a beam with no gravitational acceleration. The displacement due to the beam fall, Δy_1 is approximately,

$$\Delta y_1 = -\frac{gt^2}{2} = -\frac{gF_1^2}{2v^2} = -\frac{g(m/s^2)}{2}\frac{F_1^2(m)\lambda^2(\text{A})}{3958(m)^2}. \tag{3.1}$$

Additionally, as discussed above, the change in neutron direction –gt/v also contributes to the apparent displacement of the source, Δy_2, which is approximately,

$$\Delta y_2 = \frac{gt}{v}F_1 = g\frac{F_1^2}{v^2} \quad . \tag{3.2}$$

After deflecting from the focusing mirror the total displacement due to the apparent source shift (before the mirror) is simply Mag($\Delta y_1+\Delta y_2$) where Mag is the magnification (ratio of image distance, F_2, to object distance F_1; $Mag=F_2/F_1$). However, the neutron beam continues to fall *after* reflection ($-gF_1^2 Mag^2/(2v^2)$) causing the "central ray" to have a total shift at the sample position of,

$$\Delta y_{total} \sim \frac{gF_1^2}{2v^2} Mag(1-Mag) \ . \tag{3.3}$$

It can be shown from equation 3.3, that thermal neutrons beams focused with small demagnification optics are nearly nondispersive. For example, assuming F_1~5(m), Mag~0.1, and λ~1.4 Å, then the estimated displacement from a non-gravitationally challenged neutron beam is only 1.4 μm. The estimate of equation 3.3 compares very well to ray tracing results that include gravitational effects.

From equation 3.3 it is also clear that there are several strategies that can be used to reduce the gravitational displacement of long-wavelength neutron beams: (1) Minimize Mag; (2) work near Mag=1; or (3) minimize F_1. Although equation 3.3 does a good job of predicting the behavior of the average beam position, and correctly indicates that there is a minimum dispersion for Mag~1, there are second order effects that begin to introduce problems when working near M=1 and when collecting large divergences onto the sample. We have modeled these second order effects by ray tracing for realistic geometries. We find that there is a tradeoff between best beam size and dispersion; near Mag=1 the focus can be about 80% worse (λ ~6 Å) than the geometrical prediction, whereas at Mag ~1/5, the focused beam size is within about 6% of the theoretical prediction. However for a realistic F_1 of 3m and Mag=1/5, the gravitation dispersion of a 6 Å beam is about 17 μm, whereas near Mag= 1, the dispersion is negligible.

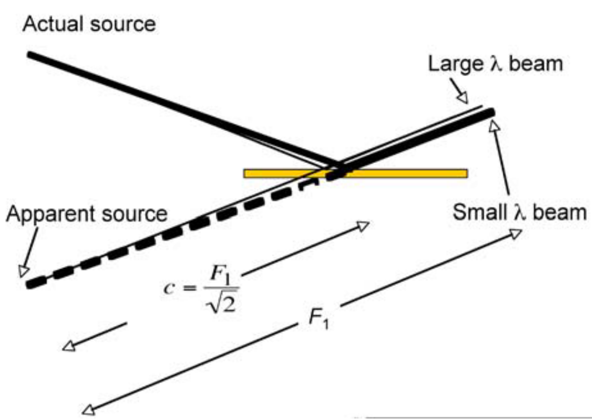

Figure 7: The apparent source point, as viewed from the vertical focusing mirror, can be made co-incident for all wavelengths when a vertically deflecting mirror is inserted at about 60% of the distance from the object to the mirror. For demagnifying optics the subsequent fall of the beam is very small and is typically less than 1 μm for realistic geometries and λ < 6Å.

One strategy to obtain best focusing *and* negligible dispersion is to precede the KB pair with a vertically deflecting mirror (Fig. 7). The apparent *source* as viewed from the vertical focusing mirror is independent of wavelength when the intermediate flat mirror is about 70% of the way from the object to the vertical focusing mirror; the apparent source displacement due to changes in beam direction exactly compensates for the actual beam fall. The final deflection of the beam at the sample is then determined purely by the fall from the mirror to the image plane, which for a realistic geometry is about two orders of magnitude smaller than the fall from the object to the mirror. Of course even this small displacement can be corrected since all deflection terms scale as gt^2; the ultimate position of the intermediate vertical deflecting mirror depends on the vertical magnification M. Ray tracing calculations based on this approach are in progress to optimize the mirror performance for various bandpass options. With this strategy it appears possible to have near ideal performance with long wavelength neutrons.

Acknowledgements are the same as the subhead style.

Research by GEI, CRH, BCL, JWLP, JDB and SS was supported by the Laboratory Directed Research and Development Program of Oak Ridge National Laboratory (ORNL) and by the Office of Basic Energy Science under contract No. DE-AC05-00OR22725 managed by UT-Battelle, LLC for the U. S. Department of Energy. SCV collaborated on measurements at the Los Alamos Neutron Science Center at Los Alamos National Laboratory. LANSCE is funded by the US Department of Energy under contract W-7405-ENG-36. RBR, JHF and RLD of the National Research Council, Canada, collaborated on experiments at the Chalk River NRU reactor. The NRU is owned and operated by AECL (Atomic Energy of Canada Ltd.) and is located at the Chalk River Laboratories of AECL, while the neutron scattering facilities are owned and operated by the National Research Council.

References

[1] D.F.R. Mildner, H.H. Chen-Mayer, W.M. Gibson, T. Gnaupel-Herold, M.E. Miller, H.J. Prask, A.J. Schultz, R. Vitt and R. Youngman, *Rev. Sci. Inst.* **73** 1985 (2002).

[2] M. Altissimo, C. Petrillo, F. Sacchetti, F. Ott, E. De Fabrizio, *Microelectronic Engineering* **73** 644 (2004).

[3] T. Oku, J. Suzuki, H. Sasao, T. Adachi, T. Shinohara, K. Ikeda, T. Morishima, K. Sakai, Y. Kiyanagi, M. Furusaka, HM Shimizu, *Nucl. Inst.& Meth*. A **529** 116 (2004).

[4] I.N. Goncharenko, I. Mirebeau, J.-M. Mignot and A. Goukasov, *Neutron News*, **14(3)** 21 (2003).

[5] P. Kirkpatrick and A.V. Baez, *J. Opt. Soc. Am,* **38** 766 (1948).

[6] G.E. Ice, C.R. Hubbard, B.C. Larson, J.W.L. Pang, J.D. Budai, S. Spooner, S.C.Vogel, *Nucl. Inst. Meth. A,* **539** 312 (2005).

[7] G.E. Ice, C.R. Hubbard, B.C. Larson, J.W.L. Pang, J.D. Budai, S. Spooner, S.C. Vogel, R. B. Rogge, J. H. Fox, and R.L. Donaberger. "High-Performance Kirkpatrick-Baez Super Mirrors for Neutron Milli- and Micro-Beams", submitted *Materials Science and Engineering A* (2005).

[8] J.R.D. Copley, *Rev. Sci. Inst.* **67** 188 (1995).