3.5.12

Preliminary study of SANS with focusing mirrors at CPHS

Huarui Wu[1], **Xuewu Wang**[1*], **Dazhi Liu**[2]

[1] Department of Engineering Physics, Tsinghua University
[2] Nuclear Reactor Laboratory, Massachusetts Institute of Technology

E-mail: * `wangxuewu@tsinghua.edu.cn`

Abstract. Axisymmetric grazing-incidence neutron focusing optics were proposed by researchers from MIT recently. We adapted these focusing mirrors to the design of SANS instruments at Compact Pulsed Hadron Sources (CPHS) which confront challenges of extremely low neutron flux. In this paper, we demonstrated one of a kind focusing mirrors: PP mirrors which consist of two coaxial paraboloids. We analyzed its geometry and we also showed the results of the ray-tracing simulations to demonstrate the performances of PP mirrors and prove that the focusing mirrors can lead to dramatic improvements for the SANS instruments based on compact neutron sources. Furthermore, different optimizations according to the desired particular improvements were discussed.

1. Introduction

The traditional Small-Angle Neutron Scattering (SANS) instruments use a collimation system which limits the size and the divergence of neutron beam[1]. Applying this traditional design to compact neutron sources would make it harder to achieve the flux we need. Therefore its significant to develop a new SANS design method especially for CPHS which is a low-energy accelerator-driver neutron source under construction in Tsinghua University[2]. Many of the techniques for focusing neutrons have been adapted from devices that have been developed for focusing X-rays[3].Inspired by the axisymmetric Wolter-type mirrors which are commonly utilized in X-ray astronomy and microscopy, the MIT group have been doing a great job to apply the idea to neutron focusing mirrors which mainly include paraboloid-paraboloid and ellipsoid-hyperboloid mirrors[1][4][5][6]. The geometrical optics of paraboloids show that neutrons emitted from the focus of a paraboloid could be reflected to be parallel and a parallel beam could be focused to the focus. Two paraboloids can be jointed up to reflect neutrons from one focus to the other as a SANS instrument implement. In this paper, we analyzed the geometry of PP mirrors to study the impact of mirrors position and radius on Q range and sample size and use a ray-tracing software package, McStas[7][8], to study the improvements of neutron flux compared with the typical SANS design[9] for CPHS when equipped with single-layer PP mirrors.

2. Geometrical analysis

The schematic layout of a SANS instrument equipped with PP mirrors is shown in Figure 1. PP mirrors consist of two parts, the left part and the right part are a section of a Paraboloid respectively. We define the Z position of the intersection which is Z_i in Figure 1 as the position of axisymmetric PP mirrors and we use the radius of the intersection R_i to represent the radius of mirrors.

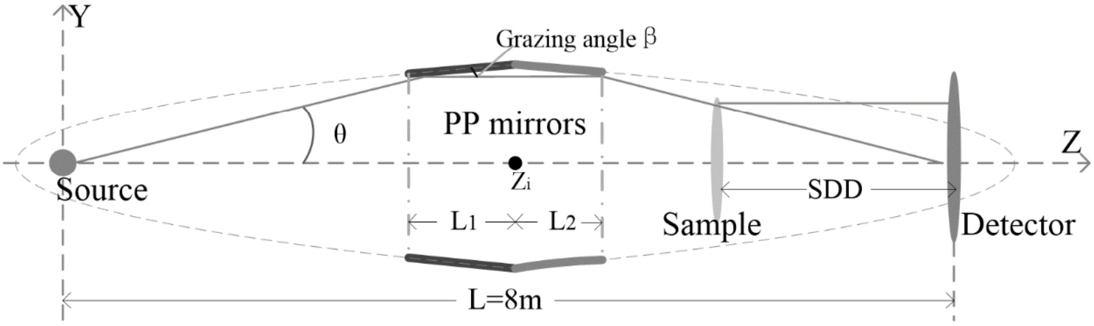

Figure 1. Schematic layout of a SANS instrument with PP mirrors. L denotes the distance from source to detector. L_1 is the length of left part and L_2 is the length of right part. SDD denotes the distance from sample position to detector position. θ is the angle between incident rays and optical axis Z while β is the grazing angle between the rays and mirrors.

Set L_1=0.6m and neutron source is monochromatic whose wavelength is 5 $\mathring{A}$. When Z_i and L_1 is determined, the magnification M of the optical system and L_2 are also determined:

$$M = \frac{L - Z_i}{Z_i} = \frac{L_2}{L_1} \tag{1}$$

The instrument equipped with PP mirrors is such a optical system in which the source represents the object and the spot in detector is the image. The radius of image R_{spot} is decided by M and source radius R_{source}, $R_{\text{spot}} = M \times R_{\text{source}}$. Many SANS experiments require reaching the smallest possible $Q(Q_{\min})$ which is one of the key performances of SANS instruments. We derived mathematical expressions for $Q_{\min}$ in our new system:

$$Q_{\min} = \frac{2\pi}{\lambda} \frac{M R_{\text{source}}}{\text{SDD}} \tag{2}$$

L_1, R_i and Z_i practically determine the mirrors ability to focus neutrons. The neutron flux increases as the increasing of R_i and thus we want to enlarge the mirrors as possible as we can. But R_i is limited by neutrons total reflection. Neutrons reflect twice in PP mirrors and only when both the reflections are total reflections can neutrons focus on the detector plane, thus the grazing angles should be smaller than the critical grazing angle which is satisfied by $\beta_c = 0.099\lambda$ in Ni mirrors. We derived mathematical expressions for grazing angle β_1 in left mirror and grazing angle β_2 in right mirror when neutrons are emitted from neutron source (0,0) and reflect in (Z_{10}, Y_{10}) firstly:

$$\beta_1 = \arctan\left(\frac{1}{\sqrt{1 + \frac{2Z_{10}}{p_1}}}\right) \tag{3}$$

$$\beta_2 = \arctan\left(\frac{1}{\sqrt{1 + \frac{2Z_{10}}{p_2}\frac{L-Z_i}{Z_i}}}\right) \tag{4}$$

Parameters p_1 and p_2 are determined by Z_i and R_i: $p_1 = -Z_i + \left(Z_i^2 + R_i^2\right)^{1/2}$, $p_2 = Z_i - L + \left[(Z_i - L)^2 + R_i^2\right]^{1/2}$. When $Z_i > L/2$, we proved that $\beta_2 > \beta_1$ which means R_i is determined by $(\beta_2)_{\max} < \beta_c = 0.495°$ and β_2 increases as Z_{10} decreases.

Moreover, sample size is a particular factor we need to consider about. In most of the SANS experiments, sample size is less than 1cm×1cm. In our new system, radius of sample is determined by R_i, Z_i and SDD: $R_{\text{sample}} \approx R_i \times \text{SDD}/(L - Z_i)$. Table 1 displays five schemes for the design of instruments with PP mirrors on the premise of sample radius less than 2cm.

Table 1. In order to set the sample radius less than 2cm, we adjusted SDD and this makes $Q_{\min}$ larger than the smallest we can achieve. Obviously, $Q_{\min}$ is smallest when we put sample on the end of PP mirrors but that would make sample as large as mirrors. I(PP)/I(No) means the ratio of the flux with PP mirrors to that without mirrors which we call traditional design and I(PP)/I(No) is calculated through simulations. The traditional configuration[9]: the source radius $R_{\text{source}} = 1.4$cm, the sampler aperture radius R_{sample}=0.5cm, SDD=5m, L=8m.

Scheme Number	M	Z_i (m)	Z_{start} (m)	Z_{end} (m)	R_i (cm)	SDD (m)	R_{sample} (cm)	$Q_{\min}$ (10^{-3}Å^{-1})	I(PP) /I(No)
1	1	4.00	3.40	4.60	6.43	1.00	1.89	17.6	3.8
2	1/2	5.30	4.70	5.60	4.44	1.00	1.85	8.8	3.5
3	1/3	6.00	5.40	6.20	3.31	1.00	1.84	5.8	1.1
4	1/4	6.40	5.80	6.55	2.65	1.00	1.83	4.4	0.54
5	1/5	6.60	6.00	6.73	2.32	1.00	1.83	3.7	0.34

According to Table 1, PP mirrors with smaller M can improve $Q_{\min}$ better but gain worse neutron intensity. SDD has no effect on intensity but has a significant impact on R_{sample}, $Q_{\min}$ and geometrical resolution. The larger SDD, the smaller sample and the better geometrical resolution we can achieve: $\Delta Q_{\text{geo}} = 4\pi M \times R_{\text{source}}/(\lambda \times SDD)$.

3. Ray-tracing simulations

We used McStas to study some key problems existing in single-layer PP mirrors. In our simulations, source radius is set to be 2.0cm. We put a source slit right after the source and the default radius is 1.4 cm. To compare with the new designs, the traditional configuration ($R_{\text{source}} = 1.4$cm, $R_{\text{sample}} = 0.5$cm, SDD=3m) was simulated. Table 1 shows the intensity ratio between instruments with PP mirrors and the traditional instruments. Its obvious that a smaller Z_i and a larger R_i could result in a higher intensity according to not only simulations but also solid angle analysis.

Table 2. Optimized R_i in different schemes

Scheme	1	2	3	4	5
M	1	1/2	1/3	1/4	1/5
Optimized R_i(cm)	5.1	4.1	3.1	2.4	2.1
I(PP)/I(No)	14.1	3.3	1.3	0.60	0.41

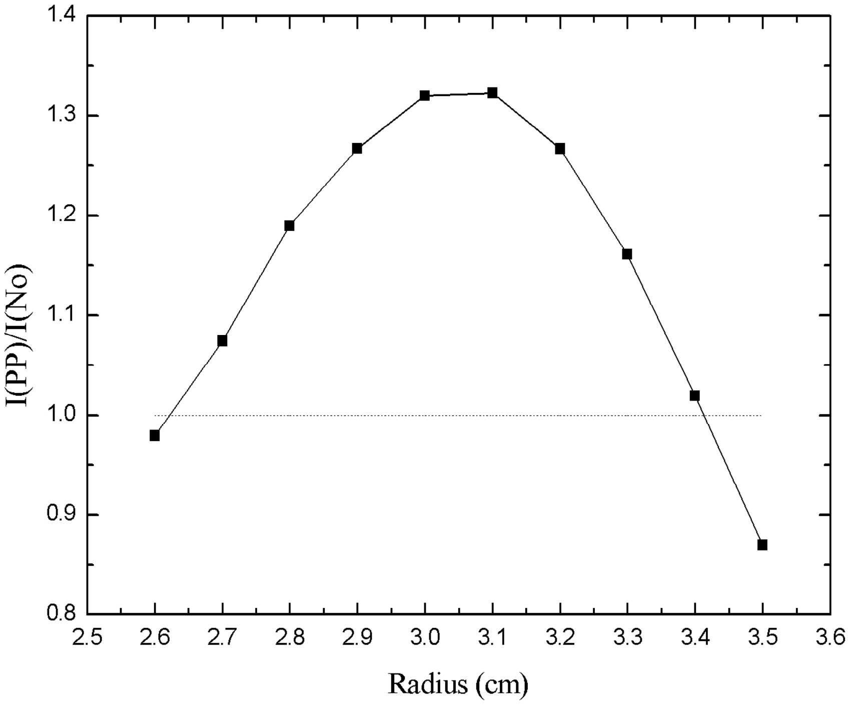

Figure 2. Intensity ratio as a function of radius of PP mirrors in scheme 2 where $M = 1/3$, SDD=1.0m.

R_i in Table 1 was calculated on the basis of point source assumption. Actually neutron source is an areal source which would cause neutrons emitted from the edge of the source may not be focused to the focal by means of two successive total reflections, so we need to adjust R_i to achieve higher intensity. Figure 2 shows the optimized R_i is smaller than that in Table 1 because of the areal sources effect. The intensity increases over 30% when R_i is set to 3.1cm compared with $Ri = 3.3$cm in Table 1. Table 2 displays the adjusted R_i of schemes from 1 to 5 in Table 1 and the adjusted ones can also decrease radius of samples.

Figure 3 demonstrates how the length of left part Paraboloid affect the neutron intensity. The results show a linear relationship between the length and intensity, and the slop increases as the M increases. The slopes of lines when M is 1, 1/2 and 1/3 are 21.87times/m, 5.25times/m and 2.20times/m respectively. So enlarge mirrors length in larger M configuration can gain neutron intensity economically. But when we want to increase neutron intensity through extending mirrors length, we should also consider if there is enough space to extend and the condition of fabrication.

Figure 4 displays the linear relationship between the neutron intensity and source radius. The slopes of lines when M is 1 and 1/3 are 9.72times/cm and 1.12times/cm respectively. According to formula (2), Q_{min} increases as R_{source} increases and decreases as M decreases. It is concluded that Q_{min} doesnt change when R_{source} increases by 2 times and M decrease by half. Comparing configuration A with $M = 1$ and $R_{\mathrm{source}} = 1.4$cm and configuration B with $M = 1/2$ and $R_{\mathrm{source}} = 2.8$cm, we find that the neutron intensity ratio of configuration A is more than 2 times than that of configuration B which tells us that a larger M and smaller R_{source} can bring better

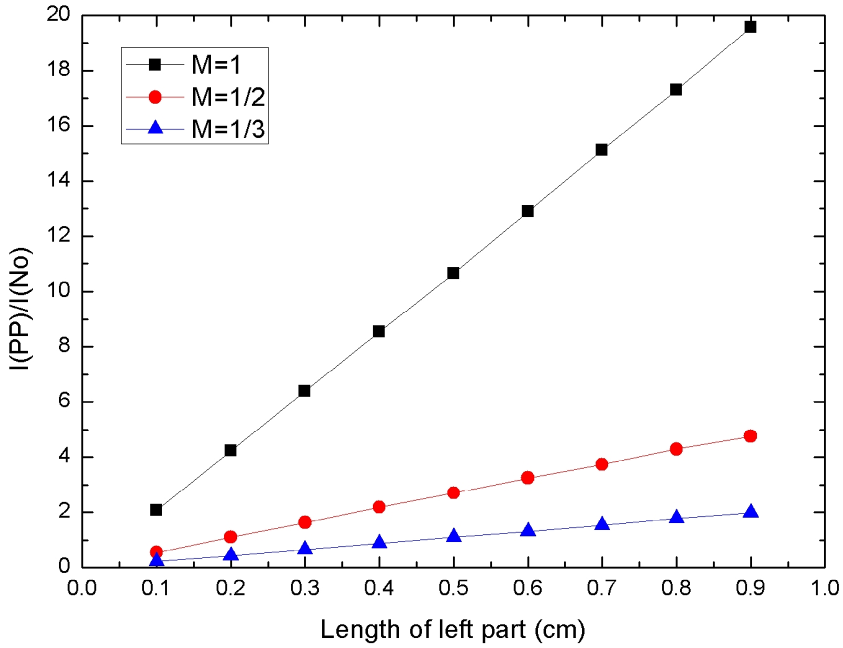

Figure 3. Neutron intensity ratio vs length of left part.

intensity and better ΔQ when we keep $Q_{\min}$ constant, but configuration A causes larger sample than other with smaller M.

4. Dissussion

The SANS instruments with different PP mirrors show different performances. The most important performances are $Q_{\min}$, ΔQ, neutron intensity and sample size is a parameter which must be considered in our new design based on focusing mirrors. Our research shows that its impossible to gain better performances in every aspects for PP mirrors but we can set the new instruments to behave very well in some particular performances to meet our needs.

For CPHS which is eagerly to increase flux, we can set M and R_i a larger value, for example, $M = 1$ and $R_i = 5.1$cm, this configuration could increase the flux by a factor of 14. But it is hard to achieve a smaller $Q_{\min}$ and a smaller sample in the same time. If we make SDD=3m, we can get a smaller $Q_{\min}$ than that in traditional design but also a very larger sample. A possible way to decrease the sample size is to employ a ring sample because the illuminating area of sample is a ring. Figure 5 displays the area of ring sample in different schemes. Setting SDD less than 1.3m can keep the area of ring sample smaller than traditional sample area. However, sample area is still more than 3 times larger than that in traditional design. And if SDD is set to less than 1.3m then $Q_{\min}$ would be nearly 2 times larger than that in traditional design. A better $Q_{\min}$ and a smaller sample size are incompatible but PP mirrors can be optional to meet different needs.

It is a great advantage for experiments using larger samples to gain much higher flux with smaller $Q_{\min}$ when M and SDD are larger and PP mirrors are nested. Nested multilayer mirrors increase the collection area by the placement of co-axial mirrors one inside another, as routinely

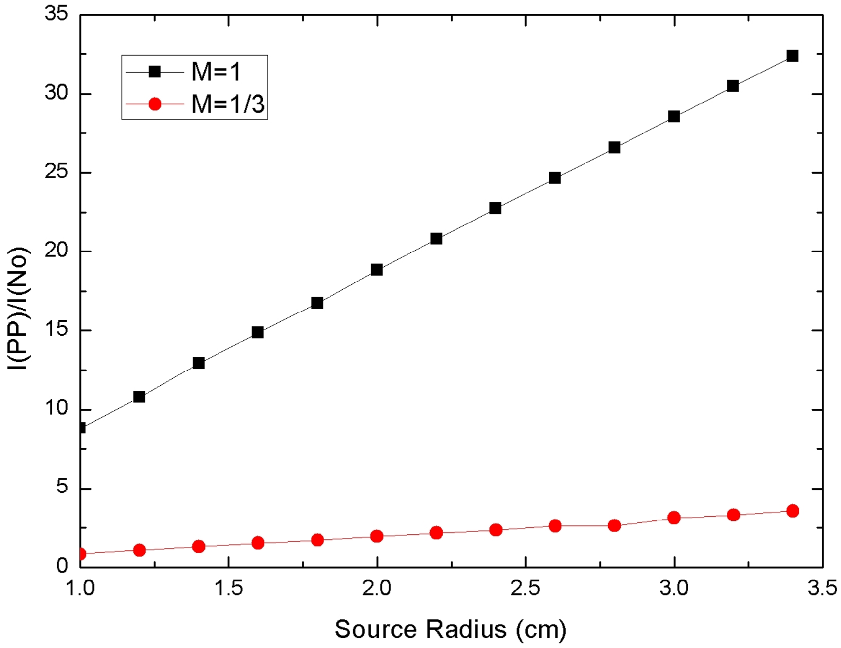

Figure 4. Neutron intensity ratio vs source radius.

done in X-ray astronomy[4]. It is estimated that a four-layer PP mirrors could increase flux by a factor of 50.[1] The construction of such a SANS instrument at CPHS specially aim at those experiments easy to employ larger sample.

Otherwise, the design with PP mirrors can also apply to improve $Q_{\min}$ when flux is not so important. When $M = 1/5$ and SDD = 1.3, $Q_{\min}$ can be decrease 2.5 times. In this case, we need a high-resolution detector and we are planning to choose MCPs to complete it.

Also, a balanced design is available when we use nested mirrors with $M = 1$, SDD=2, and R_i less than 4cm or other settings. When we adopt nested mirror into our design, higher neutron intensity is easy to achieve so that we can have better choice to improve other performances.

5. Conclusion

We demonstrate a design with focusing PP mirrors based on CPHS both in geometrical calculations and McStas simulations. SANS instruments with PP mirrors can be improved in flux and $Q_{\min}$ which is very important to SANS experiments. With larger samples, it is easy to increase neutron flux by a factor of 50. PP mirrors can also help us to extend $Q_{\min}$. These transformative improvements have great potential to change the traditional design economically and put many research into a higher stage.

PP mirrors can be used in neutron image, too. We still have much work to optimize it and its fabrications is still worth studying. We are aiming to construct the first SANS instrument equipped with such focusing mirrors and make CPHS perform better function.

---

[1] The radius of four layers are 5.8, 5.1, 4.6 and 4.0 respectively.

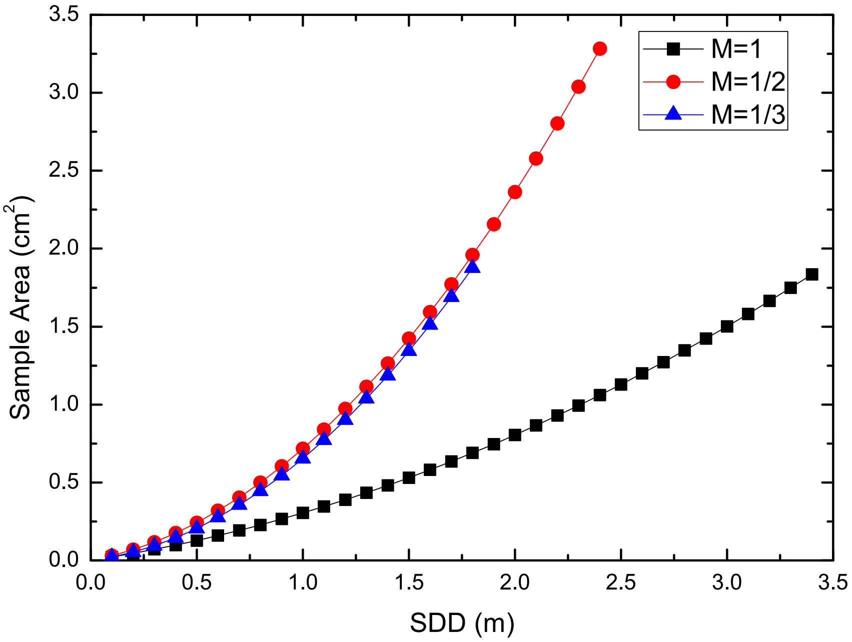

Figure 5. Relations between sample area and SDD when samples are made into rings.

6. Acknowledgement

We are grateful to Dr.Boris Khaykovich of Massachusetts Institute of Technology. This work was supported by the National Natural Science Foundation of China (No. 11322548).

References

[1] Liu D, Gubarev M V, Resta G, Ramsey B D, Moncton D E and Khaykovich B 2012 *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment* **686** 145–150
[2] Wei J, Bai Y, Cai J, Chen H, Cheng C, Du Q, Du T, Feng Z, Gong H, Guan X *et al.* 2010 *IPAC* **10** 633
[3] Mildner D and Gubarev M 2011 *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment* **634** S7–S11
[4] Khaykovich B, Gubarev M, Bagdasarova Y, Ramsey B and Moncton D 2011 *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment* **631** 98–104
[5] Liu D, Khaykovich B, Gubarev M V, Robertson J L, Crow L, Ramsey B D and Moncton D E 2013 *Nature communications* **4**
[6] Liu D, Hussey D, Gubarev M, Ramsey B, Jacobson D, Arif M, Moncton D E and Khaykovich B 2013 *Applied Physics Letters* **102** 183508
[7] Lefmann K and Nielsen K 1999 *Neutron news* **10** 20–23
[8] Willendrup P, Farhi E and Lefmann K 2004 *Physica B: Condensed Matter* **350** E735–E737
[9] Huang T, Gong H, Shao B, Wang D, Zhang X, Zhang K, Wei J, Wang X, Guan X, Loong C K *et al.* 2012 *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment* **669** 14–18