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USING THE MCLIB LIBRARY: SMALL-ANGLE INSTRUMENT WITH FOCUSING-MIRROR COLLIMATION

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Focusing mirrors in 1 or 2 dimensions can be used to increase the intensity in a small-angle instrument while maintaining high resolution. Using the recently added toroidal mirror region type in MCLIB (Monte Carlo library for neutron instrument design), we compare five mirror shapes: the ideal ellipsoid, the tangent toroid, 8 tangent toroidal segments, 8 tangential cylindrical segments, and 20 tangential cylindrical segments. A small-angle scattering instrument on a spallation source was simulated to study resolution. Comparisons show that the ellipsoid provides superior resolution, but that the 8 tangential toroids are a good compromise. A resolution of $0.00056 \text{ \AA}^{-1}$ (rms), or $\pm 11\%$ at $Q = 0.005 \text{ \AA}^{-1}$, was achieved in the simulation using neutrons in the wavelength range 4–15 Å. The count rate is high because the full area of the moderator is viewed. The latest release of the MCLIB source code and documentation may be obtained by anonymous ftp from <ftp://azoth.lansce.lanl.gov/pub/mclib/>. Work is also continuing on a friendly web-based user interface, which can be found at <http://bayberry.lanl.gov/lansce/Welcome.html>. User input is being sought for improvements to the library and to the interface.

1 Introduction

Focusing mirrors in 1 or 2 dimensions can be used to increase the intensity in a small-angle instrument while maintaining high resolution (*e.g.*, better than $Q_{\min} = 0.001 \text{ \AA}^{-1}$)^{1,2}. A small-angle scattering instrument on a spallation source was simulated with MCLIB³ to study resolution. The authors of ref. 1 used small-angle scattering with one-dimensional focusing as an example, but the same arguments concerning solid-angle matching can be applied in two dimensions using an ellipsoidal rather than cylindrical mirror. Toroids are also considered as approximations to the ellipsoid^{2,4}. Mirror shapes to be compared include the ideal ellipsoid, tangential toroidal segments, and tangential cylindrical segments.

2 The Instrument

The instrument is shown schematically in Fig. 1. The moderator is coupled liquid H₂, as proposed for the upgrade at the Manuel Lujan Jr. Neutron Scattering Center. Three choppers have been included: a T0 chopper to remove the high-energy pulse,

a frame-overlap (tail) chopper, and a frame-definition chopper which allows different wavelength ranges to be selected. In these simulations the range was 3.5–15.0 Å, at a 20-Hz pulse rate and full instrument length of 16 m. The 2-mm diameter aperture is at one focus of the ellipsoid and the detector is placed at the other focus. The mirror is 4.00 m long and 100 mm wide, with a major axis of 9.142 m and transverse (minor) axes of 239 mm, inclined 1.5° upward. The aperture and the detector are each 4.517 m from the mirror center, and the total bend angle is 3° (upward to correct for gravity⁴). The sample is 54-mm square and is located 2.50 m in front of the detector. Three “scatterers” were simulated: no sample, to observe the beam spot shape and statistics; a δ -function at $Q = 0.005 \text{ Å}^{-1}$ to compute instrument resolution directly; and hard spheres of radius 1000 Å, to illustrate data quality. For the latter two systems, the detector was recorded in 1-mm square pixels with an rms encoding error of $\pm 0.5 \text{ mm}$.

Figure 1. Layout of small-angle scattering instrument with focusing mirror. Transverse dimensions are exaggerated compared to longitudinal.

Five mirror configurations were compared. First is the ellipsoid itself, which was defined as a single surface but may also be simulated as separate segments to study the effects of misalignments. Since toroids may be easier to fabricate, the toroid tangent to the ellipsoid at its center was run next. Then a segmented mirror with 8 toroids, independently tangent to segments of the ellipsoid, was considered. To test if the second order bend of the toroids is necessary, a mirror of 8 cylinders was tested. This was so poor an approximation to the ellipsoid that a mirror with 20 cylindrical segments was also computed.

3 Results

The results for the beam spot shapes are shown in Fig. 2. Each run represents an integrated proton beam of 6.7 MW-s, which was 10^6 detected neutrons in the

Figure 2. Beam spot profiles. Upper: Ellipsoid, Toroid, 8 Toroids. Lower: 8 Cylinders, 20 Cylinders. Figures are approximately twice actual size. The intensity scale is logarithmic.

ellipsoid case. The rms values of the beam spots and also the resolution at $Q = 0.005 \text{ \AA}^{-1}$ are given in Table 1, which also has a figure of merit (FOM) based on intensity divided by variance. Comparisons of the resolution and of the data for $R = 1000 \text{ \AA}$ show that the ellipsoid is clearly superior, but that the 8 tangential toroids are a good compromise (if easier to construct). A resolution of $0.00056 \text{ \AA}^{-1}$ (rms), or $\pm 11\%$, was achieved using neutrons in the wavelength range 4–15 $\text{\AA}$.

Table 1: Resolution Results at $Q = 0.005 \text{ \AA}^{-1}$

Mirror	rms X (mm)	rms Y (mm)	rms Q ($\text{\AA}^{-1}$)	FOM
Ellipsoid	0.56	0.56	0.00056	3.43
Toroid	0.80	1.34	0.00081	1.87
8 Toroids	0.62	0.82	0.00057	3.31
8 Cylinders	1.16	5.72	0.00222	0.30
20 Cylinders	0.75	3.17	0.00115	1.08

4 Obtaining the MCLIB Code

The latest release of the MCLIB source code and documentation may be obtained

by anonymous ftp from <ftp://azoth.lansce.lanl.gov/pub/mclib/>. Work is also continuing on a friendly web-based user interface⁵, which can be found at <http://baybery.lanl.gov/lansce/Welcome.html>. You can get more information about the project by clicking on "Click here for more information" near the bottom of that page. There will be a library of standard elements which you assemble into an instrument. You then download a file containing all of the information in the proper format for input to the program MC_RUN (which you also download), and make the actual Monte Carlo run on your own computer. User input is being sought for improvements to the library and to the interface. Comments and suggestions can be sent to the author by e-mail to PASeeger@aol.com.

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