Design And MC Simulations Of A Short Wavelength Focusing Guide System For The Single Crystal Diffractometer TOPAZ At SNS

SNS — A U.S. Department of Energy multilaboratory project — Spallation Neutron Source

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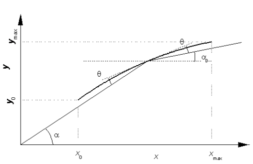
Abstract: A tapered, sectioned, focusing super mirror guide is under consideration for the Single Crystal Diffractometer (Topaz - SCD) is under development for the Spallation Neutron Source (SNS) at the Oak Ridge National Laboratory. The total incident flight path is 18 m. The IDEAS MC ray tracing package was used to simulate the neutron transport through the guide system and flux at the sample position. The guide is being designed to enhance the neutron flux starting at roughly 0.4 A and approaching its maximum gain factor of 4.8 at 1.5 A. The guide gain remains constant in the first frame up to 4 A. The last 2 m of the guide will be removable to allow for more flexibility enabling high resolution measurements or other beam focusing devices like a K-B mirror or polarizing optics. **Keywords: Focusing Neutron Guide, Neutron Instrumentation**

Arguments

- The new generation of time-of-flight [TOF] instruments needs novel design features for the neutron scattering studies involving small sampling volumes.
- The neutron guides, with constant rectangular cross section, are the basic components for transporting neutrons over large flight paths, but tapered guide section can be used as a way of spatially focusing the neutron beam.
- Monte-Carlo simulations of tapered guide sections are available in different packages as: RESTRAX, McSTAS, VITESS and IDEAS; by using these computing tools alone it is almost impossible to design an optimal guide configuration for a specific instrument.
- The ideas for focusing must be developed first, before optimizing the design via Monte Carlo simulations.

Designing a Focusing Guide

- The problem can be formulated in the following way: *how to design the end of the guide to obtain a maximum angular aperture for the neutrons coming at the sample position, in the center of the beam?*



$\alpha = \frac{y}{x} \Rightarrow \theta = -x\frac{d\alpha}{dx}$

Logarithmic Shape

- One possibility is to keep the reflection angle at a constant value:

$$\theta = \theta_0$$

- The curve having such property fulfills a logarithmic equation:

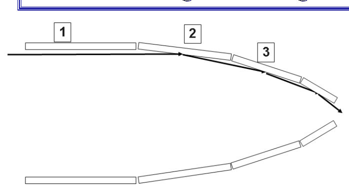
$$\frac{y}{y_{max}} = \left[1 - \frac{\theta_0}{\alpha_{min}} \ln\left(\frac{x}{x_{max}}\right)\right]\frac{x}{x_{max}}$$

- The resulting equation for α shows that the angular aperture can be increased indefinitely while x approach to 0:

$$\alpha = \alpha_{min} - \theta_0 \ln\left(\frac{x}{x_{max}}\right)$$

I.N. Goncharenco, I. Mirebeau, J.-M. Mignot and A. Goukasov, Neutron News, 12,3, 21-24, 2003. *Neutron diffraction on microsamples under high pressures*

Piecewise Design of a Focusing Guide



Multiple-stage tapered guide system – the continuous mirror replaced with a sequence of straight segments

A.D. Stoica, X.-L. Wang, W.-T. Lee and J.W. Richardson, in *Advances in Computational Methods for X-Ray and Neutron Optics, Denver, 2004*, edited by Manuel Sanchez del Rio, Proceedings of SPIE Vol. 5536 (SPIE, Bellingham, WA, 2004), p. 86.

Design Considerations

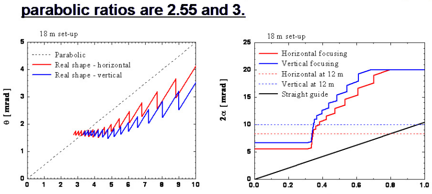
- **As the spatial focusing effect is obtained by increasing the angular divergences, the design of any particular instrument should take into account the implicit worsening of resolution. We should start from a desired beam cross-section at the end of the guide, which is essentially determined by the worst accepted resolution.**
- **A controlled variation of the reflection angle along the guide can be allowed in order to shape a smoother angular distribution and wavelength dependence. A first part of the guide will still follow a logarithmic shape, but in the following parts a steady variation of the reflection angle, proportional to the divergence angle, will be allowed. As the ratio between a and q will be higher then 2, we name this kind of curves super-parabolic.**

Requirements

- **The primary objective was to design a guide system for a 18 m primary flight path, that will preserve the flux on sample and divergence of a primary flight path of 12 m. The divergence for this distance of a 100 mm x 120 mm moderator view is approx. 10 mrad.**
- **A simple straight guide cannot fulfill this demand, as the critical angle decreases dramatically for neutron wavelengths smaller then 1 Å. A focusing guide can increase the angular divergence for short wavelengths. However, the lower limit would be set by the range of the critical angle allowed by the guide profile. We choose this limit at 0.4 Å.**
- **A second design goal was to explore the possibility of increasing the angular divergence up to 20 mrad, or even 30 mrad, for high intensity measurements. Our search shows that a 20 mrad set-up would be possible to design by using a single-channel guide system. However, the only way to increase the divergence over this limit would be to replace the last part of the guide with a system of two concentric tapered guides.**
- **As the distance from the guide end to the sample position was fixed to 0.5 m, the cross section of the exit should be 10×10 mm to allow a maximum divergence of 20 mrad in the horizontal and the vertical planes. The guide entrance was set at 6 m away from the source. Therefore, the total length of the guide would be 11.5 m. The source cross- section is 100×120 mm and, consequently, the guide cross section at the entrance should be smaller then 67×80 mm. If the cross section exceeds these limits, gaps in the angular distribution at the sample position would appear.**
- **The 11.5 m guide has 15 sections. The shortest is 20 cm long and will be placed at the end of the guide.**

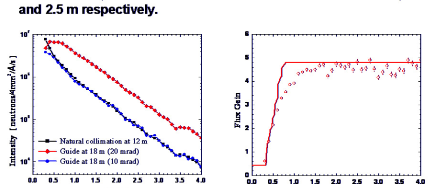
Optimizing guide profile

- **The guide profile was calculated to allow a maximum super-parabolic ratio starting from a minimum constant reflection angle of 1.75 mrad. Horizontal/vertical super-parabolic ratios are 2.55 and 3.**



MC – intensity

- **At about 0.4 Å the guide delivers the same divergence as the natural collimation at 12 m. At about 0.8 Å, the divergence reaches a maximum 20 mrad. To restrict the divergence to 10 mrad, three slits of 5 mm, 10 mm and 25 mm should be inserted at 0.5 m, 1 m and 2.5 m respectively.**



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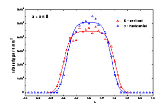
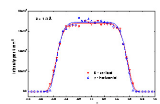
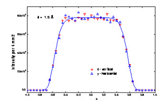
MC – angular divergence (1)



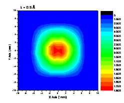
- 20 mrad option:

λ [Å]	Vertical FWHM [mrad]	Horizontal FWHM [mrad]
0.5	13.9	12.1
1.0	19.3	19.0
1.5	19.7	19.7



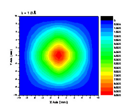


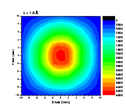
MC – beam cross section (1)



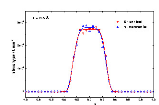
- 20 mrad option:

λ [Å]	Vertical FWHM [mm]	Horizontal FWHM [mm]
0.5	8.0	8.3
1.0	9.5	9.0
1.5	11.5	12.1



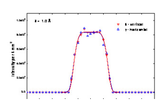


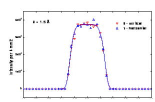
MC – angular divergence (2)



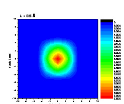
- 10 mrad option:

λ [Å]	Vertical FWHM [mrad]	Horizontal FWHM [mrad]
0.5	8.9	8.7
1.0	9.2	9.2
1.5	9.2	9.2



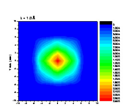


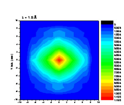
MC – beam cross section (2)



- 10 mrad option:

λ [Å]	Vertical FWHM [mm]	Horizontal FWHM [mm]
0.5	5.9	5.6
1.0	6.6	7.5
1.5	6.6	8.1





Conclusions

- **The reflection angle of neutrons crossing the beam axis at sample position seems to be the main parameter for flux density maximization. The profile of a focusing guide can be designed by optimizing the correlation between the reflection angle and the corresponding divergence angle.**
- **The optimal solution is fully determined by the dimensions of the guide at its entrance and at its end. These dimensions have to be determined from other criteria.**
- **The focusing guides can significantly increase the flux density at the expense of reducing the beam cross section. This concept works even for short wavelengths (1 Å or less).**
- **The focusing guides in combination with a convergent collimator can reduce the sampling volume for the diffraction down to a sub-millimeter size, while keeping the angular acceptance to a high level (10-30 mrad).**