Advances in instrument design for single crystal diffraction at SNS

C. Hoffmann[1], A. Stoica[1], H. Lee[1], X.-L. Wang[1], A. Schultz[2], P. B. Piccoli[2], T. Koetzle[2,3], R. Bau[3], J. Thomison[1], L. Davis[1]

[1]Oak Ridge National Laboratory, Oak Ridge, TN, [2]Argonne National Laboratory, Argonne, IL, [3]Brookhaven National Laboratory, Upton, NY, [4]University of Southern California, Los Angeles, CA

Abstract: A Single Crystal Diffractometer (Topaz - SCD) is under development for the Spallation Neutron Source (SNS) at the Oak Ridge National Laboratory. It will make possible high speed data collections on samples that will approach the size of a typical X-ray crystal. This requires to efficiently transport the neutron beam from the moderator to the sample position without increasing the beam divergence drastically. The instrument design takes into account a baseline divergence of 10 mrad similar with a much shorter 12 m instrument. To conserve the flux and divergence starting at 0.4 Å efficiently a tapered, sectioned, focusing super mirror guide is under consideration [1]. Monte Carlo simulations of the neutron transport through the guide system and flux at the sample position were carried out using the IDEAS MC ray tracing package [2]. The guide geometry enhances the neutron flux starting at roughly 0.4 Å, approaching its maximum gain factor of 4.8 at 1.5 Å. The guide gain remains constant in the first frame up to 4 Å. A series of variable slits within the last two meters of the guide exit enable a high flux and high resolution option. The last 2 m of the guide will also be removable to allow for more flexibility enabling high resolution measurements or to switch to other beam focusing devices like a K-B mirror[3] or polarizing optics [4]. Currently, the instrument is scheduled to be completed by 2009.

[1] 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.

[2] W.-T. Lee and X.-L. Wang, Neutron News 13, 30 (2002).

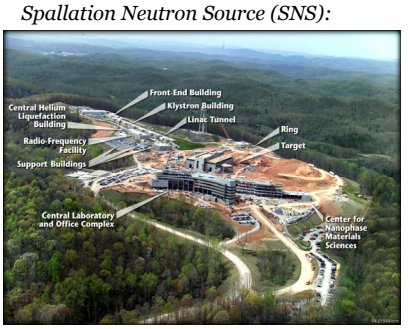
[3] G.E. Ice, C.R. Hubbard, B.C. Larson, J.W.L. Pang, J.D. Budai, S. Spooner and S.C. Vogel, Nucl. Inst. Meth. Phys. Res. A 539, 312 (2005).

[4] G.L. Jones et al., Continuously operating compact 3He-based neutron spin filter, Acta Phys. B, Vol. 356 (Proc. of the 5th Int'l. Workshop on Polarized Neutrons in Condensed Matter Investigations, Washington 2005), p. 86, (2005).

Keywords: Single Crystal Neutron Diffraction, Focusing Neutron Guide, Neutron Instrumentation

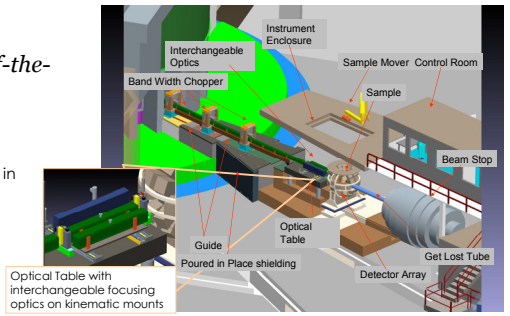
- The SNS is under construction at the Oak Ridge Nat'l. Laboratory
- TOPAZ is part of SING (SNS Instruments – Next Generation)
- The SNS will begin operation in 2006
- At 1.4 MW it will be ~8x ISIS, the world's leading pulsed spallation source
- The peak neutron flux will be ~20–100x ILL
- SNS will be the world's leading facility for neutron scattering
- It will be a short drive from HFIR, a reactor source with a flux comparable to the ILL

Spallation Neutron Source (SNS):



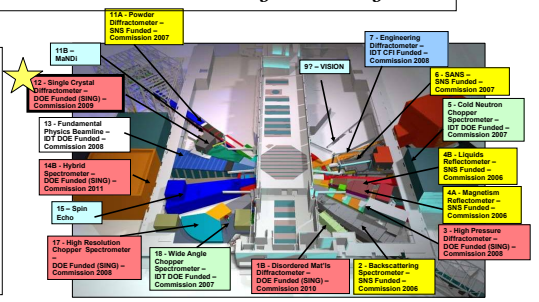
Instrument Design Implements State-of-the-art Neutron Beam Transport

A highly reflective guide system in the incident flight path with interchangeable guide and focusing sections for the last 2 m before the sample to focus the beam between ~$(100\mu m)^2$ < a < $(2mm)^2$.



Instrument Location in the SNS Target Building:

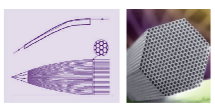
TOPAZ-SCD on Beamline 12 (upper decoupled cold H-moderator) is currently at detailed engineering design and beginning construction stage.

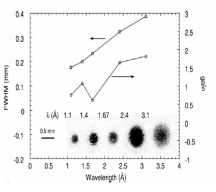


The instrument design concept as a 3-D model is depicted above. The optical table just upstream of the sample-detector mounting system holds interchangeable beam focusing options. A highly reflective guide system with interchangeable focusing options before the sample optimizes the neutron beam to probe single crystal volumes 100mm <v<2mm.

- The final focusing neutron beam guide section for beam cross section of 2mm x 2mm @ 1 Å is described on the right.
- The micro-focusing optic for beam cross section ~ 100μm x 100μm @ 1 Å is described below.

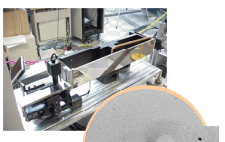
1) Glass fiber based poly capillary optic (courtesy of XOS, Albany, NY)[1] using total external reflection to transport the neutron beam

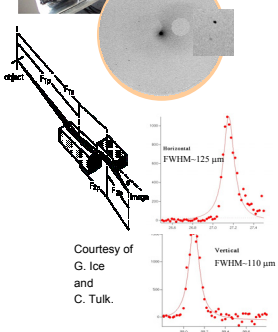




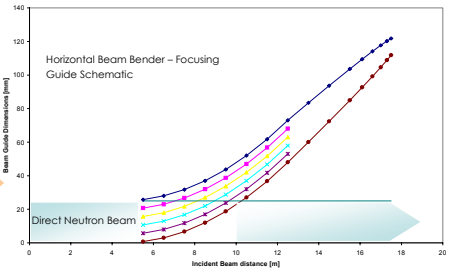
[1]Gibson et al., Polycapillary focusing optic for small-sample neutron crystallography, J. Appl. Cryst. 35, 677-683, 2002.

2) Highly reflective surface Kirkpatrick-Baez mirrors reflecting the beam off a elliptically curved super-mirror surface

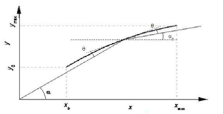




Courtesy of G. Ice and C. Tulk.



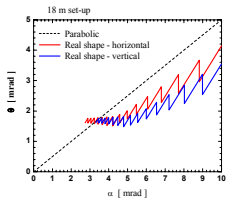
Designing a Focusing Guide Determined by Divergence at Sample and Reflection Angle

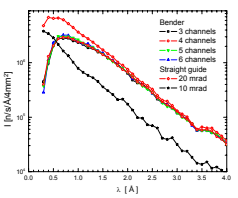


- Basic equation: $\alpha' = \frac{y}{x} \Rightarrow \theta = -x\frac{dx}{dx}$
- Ellipse / Parabola: $\frac{x_s}{\theta} = 2\left(1-\frac{x}{x_{max}}\right)$; $y = \frac{x}{x_{max}}$, m - demagnification
- Reflection angle controlled solution: spiral logarithmic $\frac{y}{y_{max}} = \left[1 - \frac{\theta_0}{\alpha_{min}} \cdot \ln\left(\frac{x}{x_{max}}\right)\right]\frac{x}{x_{max}}$

Neutron Beam Guide: Concept and Performance Evaluation by Monte Carlo Ray Tracing

Novel neutron guide design using m=3 super mirror coating (=3 x the reflectivity of natural Ni) following the trace of a "super parabolic" surface (combined logarithmic spiral & parabolic) in straight sections (piecewise approximation). The fast neutron portion of the pulsed beam is discriminated by a 5 channel bean bender. Neutrons of ~0.4 – 4 Å will reach the sample position in the first frame. Above are the beam guide system layout showing the horizontal focusing and bender (upper-left) and the guide design considerations (upper-right).



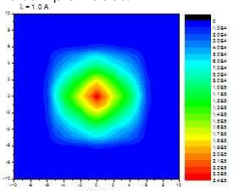


To the left MC results for this vertically continuously focusing and horizontally bending & focusing guide are shown. The divergence on sample lies between the determined limits of 10 – 20 mrad with 4.8 gain.

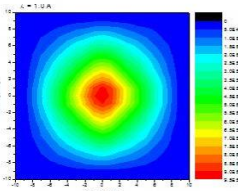
Monte Carlo Simulations[1] at the Sample Position for 4 mm²:

Modulation option from 10 mrad for high resolution to 20 mrad for high intensity on the sample to tailor measurement conditions to sample needs.

Neutron beam cross section for high resolution setting at 1 Å calculated by Monte Carlo ray tracing methods



Neutron beam cross section for high intensity setting at 1 Å calculated by Monte Carlo ray tracing methods



[1] IDEAS: MC ray tracing package, W.-T. Lee and X.-L. Wang, Neutron News 13, 30 (2002).

Acknowledgements:
SING (SNS Instruments – Next Generation) is managed by UT-Battelle, LLC, under contract DE-AC05-00OR22725 for the U.S. Department of Energy. The Authors wish to acknowledge the support of the U.S. Department of Energy Office of Science under contract No. DE-AC05-960R22464. Argonne National Laboratory was supported by the U.S. Department of Energy, Basic Energy Sciences–Material Sciences, under Contract No. W-31-109-ENG-38.

Spallation Neutron Source
www.sns.gov