ICANS-XV
15th Meeting of the International Collaboration on Advanced Neutron Sources
November 6-9, 2000
Tsukuba, Japan

12.8

Monte Carlo simulation of the neutron guide system for the SNS engineering diffractometer

X.-L. Wang and W.-T. Lee

Spallation Neutron Source, Oak Ridge National Laboratory
Building 7964H, Oak Ridge, TN 37831-6430
USA

Abstract

VULCAN, the SNS engineering diffractometer, is designed to tackle a broad range of engineering problems, from residual stress distribution in components to materials response under loading. In VULCAN, neutrons are delivered to the sample position via a series of straight and curved neutron guides. An interchangeable guide-collimator system is planned in the incident beam path, allowing the instrument to be optimally configured for individual experiments with different intensity-resolution requirements. To achieve maximum data rate and large d-spacing coverage, detectors are employed continuously from 60° to 150° in the horizontal scattering plane and -30° to 30° in the vertical plane. To enable simultaneous small angle scattering measurements for characterization of the microstructure, the instrument is also equipped with a position sensitive area detector. Monte Carlo simulation indicates that the proposed neutron guide system is able to deliver the desired intensity and resolution.

1. Introduction

At the recommendation of the SNS Instrument Oversight Committee, conceptual design work has been undertaken for an engineering materials diffractometer as a potential candidate for inclusion in the initial suite of instruments. Scientific cases for this instrument were established by the user community at a number of workshops and have been summarized in a report by Holden [1]. At the moment, the instrument is tentatively named VULCAN, after the Roman god of fire and metalworking. Although the primary use of VULCAN is intended for deformation and residual stress related studies, other uses include spatial mapping of chemistry, microstructure, and texture.

The desired performance for VULCAN as determined by the user community are listed below.

- rapid volumetric (3-dimensional) mapping with a sampling volume of 1 mm^3 and a measurement time of minutes
- very high spatial resolution (0.1 mm) in one direction with a measurement time of minutes
- ~20 well defined Bragg reflections for in-situ loading studies

- ability to study kinetic behaviors in sub seconds
- simultaneous characterization capabilities, including dilatometry, weight, and microstructure
- ancillary equipment such as furnace and load frame be an integrated part of the instrument

Together, these requirements call for a "compound" engineering diffractometer with a large degree of flexibility for intensity-resolution optimization. The design philosophy is therefore to deliver a diffractometer with the highest desirable Q-resolution over a large angular range. For experiments that do not require such a high Q-resolution, the incident beam divergence can be relaxed for intensity gain at the sample position.

2. Design concept

Fig. 1 shows the proposed baseline design. The incident beam flight path is 44 m, consisting of a 3 m in-monolith guide, a bandwidth chopper, a 20 m curved guide followed by a 12 m straight guide, and a 5 m interchangeable guide-collimator system. All guides have a cross-section of 12×50 mm^2 and 3θ_c supermirror coatings on all sides. The in-monolith guide section ensures that the neutron guides are fully illuminated. A chopper with an adjustable opening and variable operating frequency is used to define the wavelength bandwidth for VULCAN. To minimize the leak of unwanted neutrons, the chopper is placed right after the biological shielding. The long curved guide is used to suppress the transmission of high-energy neutrons. Neutrons emerging from a curved guide have an uneven spatial distribution at the exit, which is particularly pronounced at short wavelength. A straight guide section is therefore used to balance this uneven distribution. The interchangeable guide-collimator system consists of five 1 m segments, each containing two channels, which is either a 3θ_c supermirror guide or a straight collimator. Each channel can be translated into the beam position at the push of a button. These channels may be used in combinations to produce an incident beam of desirable divergence. The interchangeable guide-collimator is a key to the design, as it allows the instrument to be optimally configured for individual experiments with different intensity-resolution requirements. A 1 m space is left between the sample and the exit of the guide-collimator system. In addition to housing the incident slit unit, this space may also be used to accommodate additional shielding or collimators.

Large detector coverage is another feature of VULCAN. Traditionally, stress mapping at pulsed neutron sources were carried out using detectors in the vicinity of 90° scattering angle. However, a recent study by Wang [2] showed that detectors over a much wider angular range can all be used effectively for stress mapping. In the present design for VULCAN, the detector array covers 60°-150° in the horizontal scattering plane and ±30° in the vertical plane. The sample to detector distance is set at 3 m in order to achieve the specified Q-resolution and also to leave sufficient room for the use of optional devices such as a Bragg Mirror [3]. To enable simultaneous characterization of the microstructure, a position-sensitive area detector will be mounted downstream at 4 m from the sample so that simultaneous diffraction and small angle scattering measurements can be made. By using a small specimen (e.g., < 5 mm width), a poor-man's SANS attachment can be realized with no disruption to the base-line design. For a 60 Hz target, the estimated Q-range for SANS measurements is 0.01 Å^{-1}-0.18 Å^{-1}. When desirable, a larger Q-range can be obtained by eliminating every other pulse using the bandwidth chopper.

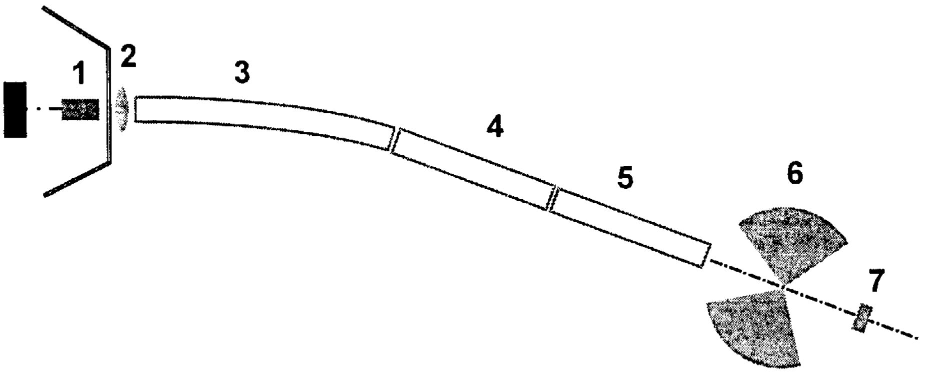


Fig. 1 Schematic of the base line design for VULCAN. The basic components and their characteristics are given below.
1 - in-monolith guide ($3\theta_c$ supermirror, 3 m)
2 - bandwidth chopper
3 - $3\theta_c$ curved guide (20 m)
4 - $3\theta_c$ straight guide (12 m)
5 - interchangeable guide-collimator system (5 m)
6 - detector banks (at 3 m to sample, 60°-150° in the horizontal scattering plane and ±30° in vertical plane)
7 - SANS detector (4 m from sample)

3. Monte Carlo Simulation

Monte Carlo simulation was used to evaluate the performance of the neutron guide system. The simulation work was carried out using IDEAS® (**I**nstrument **D**esign and **E**xperiment **A**ssessment **S**uite), a general-purpose software package developed at the Oak Ridge National Laboratory for simulating the optics of neutron scattering instruments. The simulation program utilizes a linear approach illustrated in the schematic flow-chart in Fig. 2. Self-contained subroutine modules, each of them simulating the interaction of a neutron with a particular optical element, e.g., a guide section, are arranged in a series to form an instrument. During a simulation, a set of parameters that specifies the state of a neutron is passed sequentially to the series of modules. Each module modifies the neutron parameters subject to the physics of the interaction. The codes of the subroutine modules in IDEAS® are pre-compiled into shared libraries. At run time, the relevant pre-compiled modules are linked dynamically into the simulation loop and the parameters for each optical element are imported and passed to the module. The use of pre-compiled modules and the dynamic loading of information allows rapid prototyping of an instrument since, upon setting up or changing an instrument's configuration, the simulation can readily begin without the intermediate step of recompilation. An integrated user interface explained below reduces the work for the inclusion/deletion of a module and the change of a module's parameters to virtually the click of a button, thus allowing a user to focus on the instrument parameters and its performance and rather on the convention of the specifications. IDEAS® has also adopted a standardized specifications for both the neutron parameters and the subroutine interface structure, therefore not only ensuring a smooth passage of data between the modules, but also guaranteeing the reusability of existing modules and the easy incorporation of new modules into the suite.

The user interface for IDEAS® was implemented on the Windows platform using the Microsoft® Visual C++ integrated development environment. An example illustrating the use of this interface is shown in Fig. 3. On the left is a window containing a list of available modules, which are generated using Microsoft Visual C++ in the form of a DLL. The window in the middle lists the sequence of modules that are selected to form a target instrument. Double clicking a module in this window opens an interface where users can set the parameters for the module. During a simulation, the neutrons propagate through the modules in the order in which they are placed in the target instrument module list. The right window is reserved for execution control, where users can decide when to terminate the run or whether to save the history files, and so on. At present, more than 30 modules are available within IDEAS®, including, for instance, neutron guides, collimators, monochromators, and powder samples.

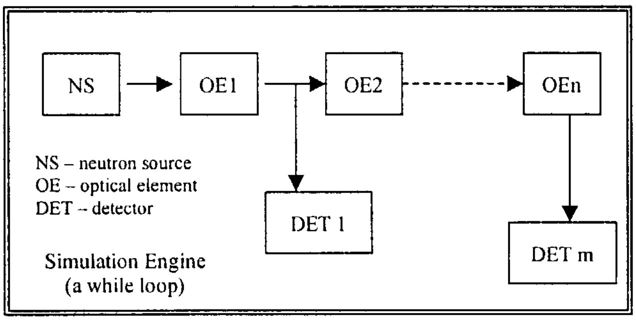
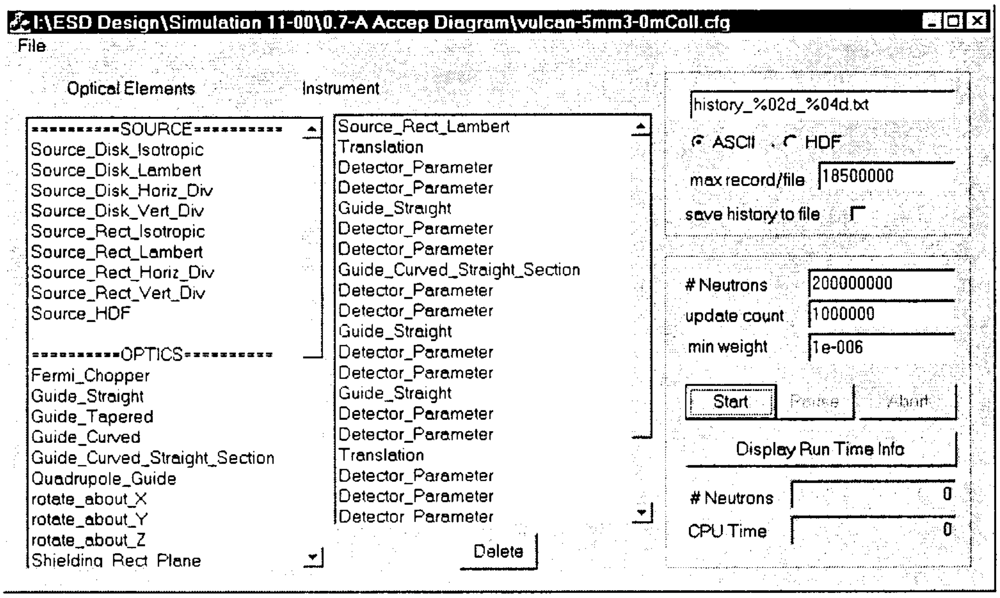


Fig. 2 A linear model used by IDEAS® for simulation of a neutron scattering instrument.



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Optical Elements:

==========SOURCE==========
Source_Disk_Isotropic
Source_Disk_Lambert
Source_Disk_Horiz_Div
Source_Disk_Vert_Div
Source_Rect_Isotropic
Source_Rect_Lambert
Source_Rect_Horiz_Div
Source_Rect_Vert_Div
Source_HDF

==========OPTICS==========
Fermi_Chopper
Guide_Straight
Guide_Tapered
Guide_Curved
Guide_Curved_Straight_Section
Quadrupole_Guide
rotate_about_X
rotate_about_Y
rotate_about_Z
Shielding_Rect_Plane

Instrument:

Source_Rect_Lambert
Translation
Detector_Parameter
Detector_Parameter
Guide_Straight
Detector_Parameter
Detector_Parameter
Guide_Curved_Straight_Section
Detector_Parameter
Detector_Parameter
Guide_Straight
Detector_Parameter
Detector_Parameter
Guide_Straight
Detector_Parameter
Detector_Parameter
Translation
Detector_Parameter
Detector_Parameter
Detector_Parameter

history_%02d_%04d.txt
● ASCII ○ HDF
max record/file 18500000
save history to file ☐

Neutrons 200000000
update count 1000000
min weight 1e-006

Neutrons 0
CPU Time 0

Fig. 3 User interface for IDEAS®.

4. Simulation results and discussions

In VULCAN, a long curved guide is used to suppress the transmission of high energy (E≥eV) neutrons at the sample position. Calculations show that for a 20 m guide with a curvature radius of 2 km, the moderator will be well out of line of sight. In general, high critical angle coating is required in order to improve the transmission of neutrons at short wavelength (e.g., 1 Å).

Fig. 4 illustrates the effect of curvature on neutron transmission. As it can be seen, high energy neutrons (E≥eV) are greatly suppressed. The transmission efficiency increases to 80% for 0.7-Å neutrons and close to 100% at 3 Å and beyond. It is anticipated that with the use of a curved guide, a T_0 chopper will not be necessary.

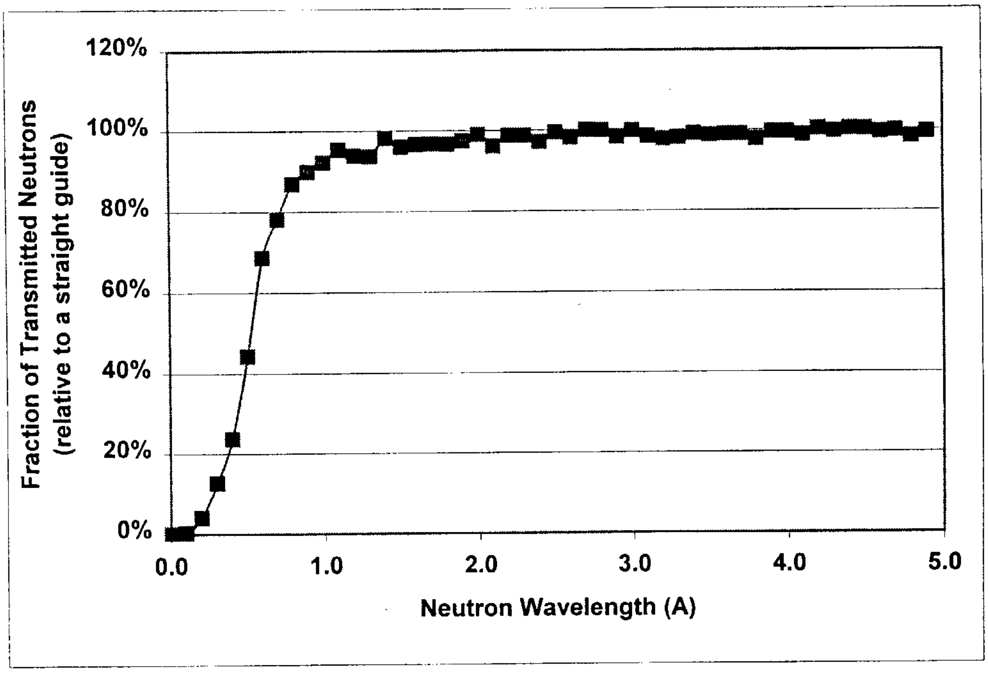

Fig. 4 Fraction of trasnmitted neutrons due to curving of a neutron guide. The guide is assumed to have a cross-section of 12×50 mm^2, a length of 20 m, and $3\theta_c$ supermirror coatings on all sides. The radius of cuvature is 2 km.

Next, Monte Carlo simulation was used to assess the influence of various guide-collimator configurations on intensity and resolution. Three configurations were investigated: (1) 5 m guide, (2) 3 m guide followed by 2 m collimation, (3) 5 m collimation. These are labeled as high intensity, 2 collimation, and high resolution mode, respectively. The simulation results are plotted in Figs. 5-6. As it can be seen from Fig. 5, the high resolution mode is accompanied with a factor of 2-5 loss in intensity. Fig. 6 shows the horizontal divergence of the incident neutron beam at the sample position. In the high resolution mode, the FWHM of the incident beam is 0.11°. Natural collimation, with a FWHM~0.06°, is reached when the guide is terminated at 10 m from the sample. Monte Carlo simulation for this configuration shows a further decrease in neutron intensity, by a factor of 2. The calculated resolution function (Δd/d) for the 90°detector is shown in Fig. 7 along with the results obtained for SMARTS (see below). A 0.2% resolution is achieved in the high resolution mode, which is sufficient to resolve ~ 20 peaks for most engineering materials such as steel, aluminum, and alumina ceramics. In the high intensity mode, the resolution varies almost linearly as a function of d-spacing, from 0.32% at 0.5 Å to 0.53% at 2.5 Å. This mode is suited for study of deformed specimens whose diffraction peaks are intrinsically broad.

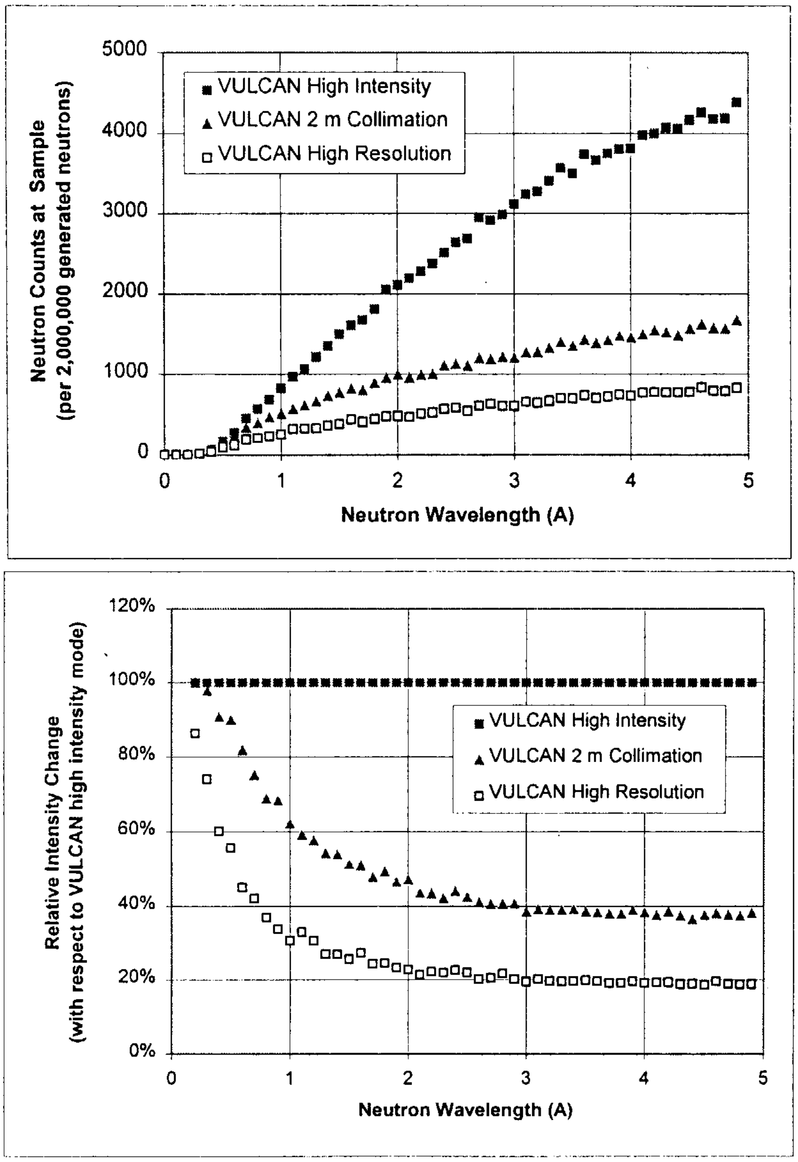

Fig. 5 Monte Carlo simulation to assess the performance of the guide-collimator system for selected operating configurations. Top panel: neutron counts at sample. Bottom panel: relative intensity change with VULCAN high intensity mode as the baseline. The neutron source is a Lambert source with a uniform flux as a function of neutron wavelength. A total of 2,000,000 neutrons were generated in each case. The sample is assumed to have a 5×30 mm^2 cross section. The bandwidth chopper was not considered in this simulation.

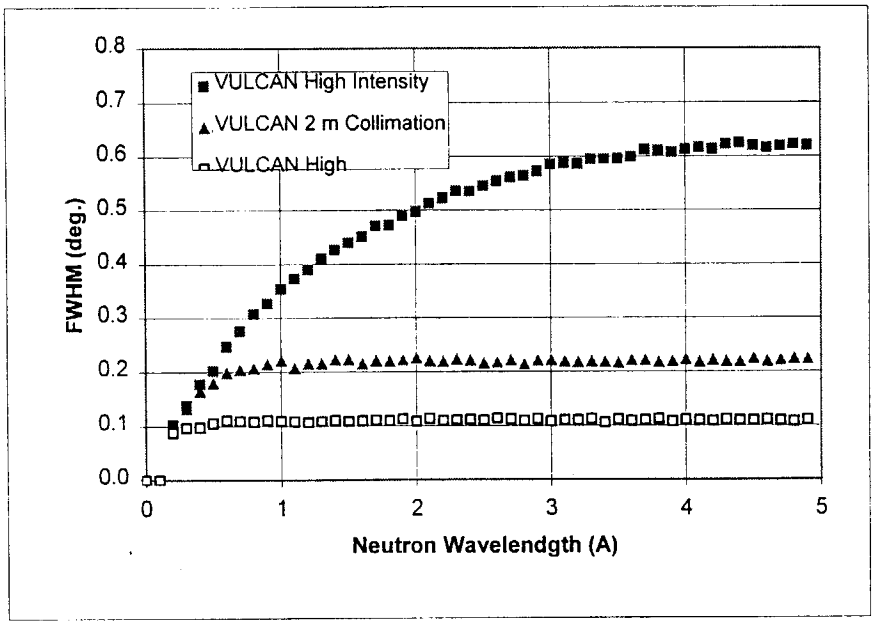

Fig. 6 Monte Carlo simulation results for the FWHM of the incident neutron beam in the horizontal scattering plane for selected operating configurations of the guide-collimator system.

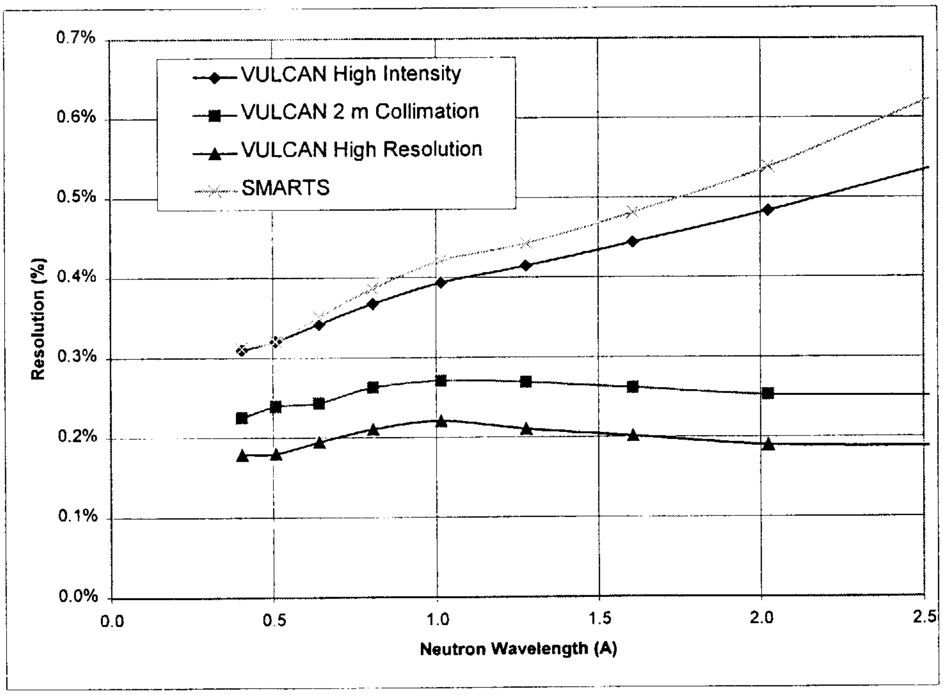

Fig. 7 Calculated resolution function for the 90° detectors. For comparison, the results for SMARTS (see text below) are also plotted.

As noted earlier, neutrons emerging from the curved guide have an uneven spatial distribution. This effect, which becomes progressively pronounced at short wavelength, can be greatly reduced if a long straight guide is used following the curved guide. Fig. 8 shows the spatial distribution for 0.7-Å neutrons across the guide width (i.e., in the horizontal scattering plane). After a 12 m of straight guide, the intensity becomes quite uniform. The maximum difference from left to right at the exit of the straight guide is less than 10%, which further diminishes after the guide-collimator system. Further analysis of the acceptance diagram (obtained from Monte Carlo simulation) confirms that the uneven spatial distribution resulting from the curved guide has largely disappeared after a 12 m straight guide.

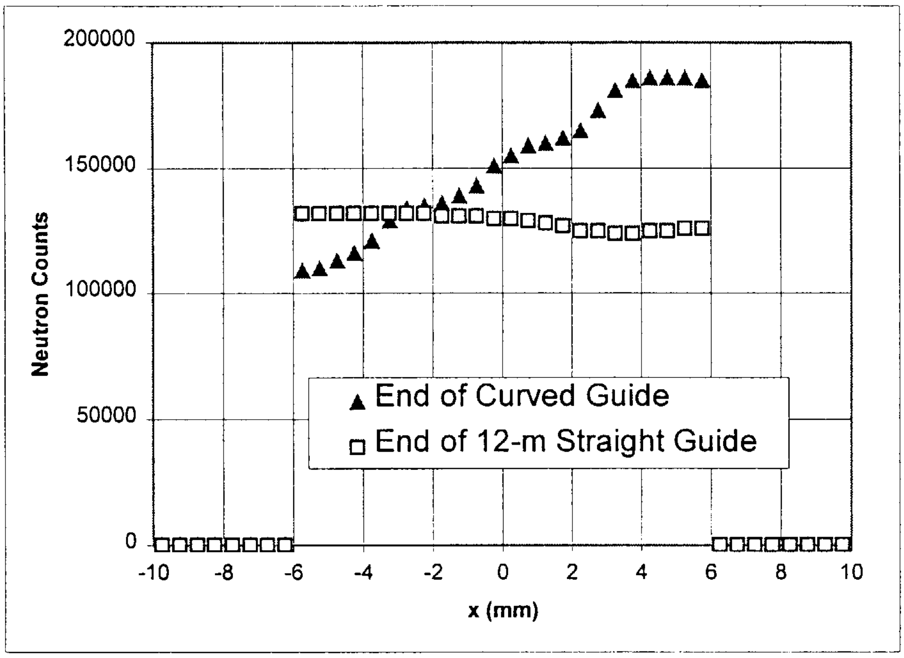

Fig. 8 Spatial distribution of neutron intensity at the beginning and end of the 12 m straight guide. The steps seen in both profiles are due to approximating the curved guide with 20 1-m segments.

The performance of the VULCAN guide design is benchmarked against that of SMARTS, a next-generation engineering diffractometer currently under construction at Los Alamos National Laboratory. There are several important differences between the neutron optical systems for SMARTS and VULCAN. SMARTS uses straight guides only, with a cross section of 50×50 mm^2. The guide system starts at 5 m from the moderator and terminates at 29 m. The guide coatings are natural Ni on the sides, and $3\theta_c$ supermirror on the top and bottom surfaces. The sample is at 30 m from the moderator. The detector to sample distance is 1.5 m.

To compare with SMARTS, a Monte Carlo simulation was performed using the design parameters as of August 1999. To assess the performance of the neutron guide system, the SAME neutron source and sample was used. As in the simulation for VULCAN, the choppers in SMARTS were ignored. The simulated neutron intensity per 2,000,000 generated neutrons is plotted in Fig. 9, along with the results obtained for VULCAN. It can be seen that with the same source, VULCAN and SMARTS have similar neutron intensity. At VULCAN's primary

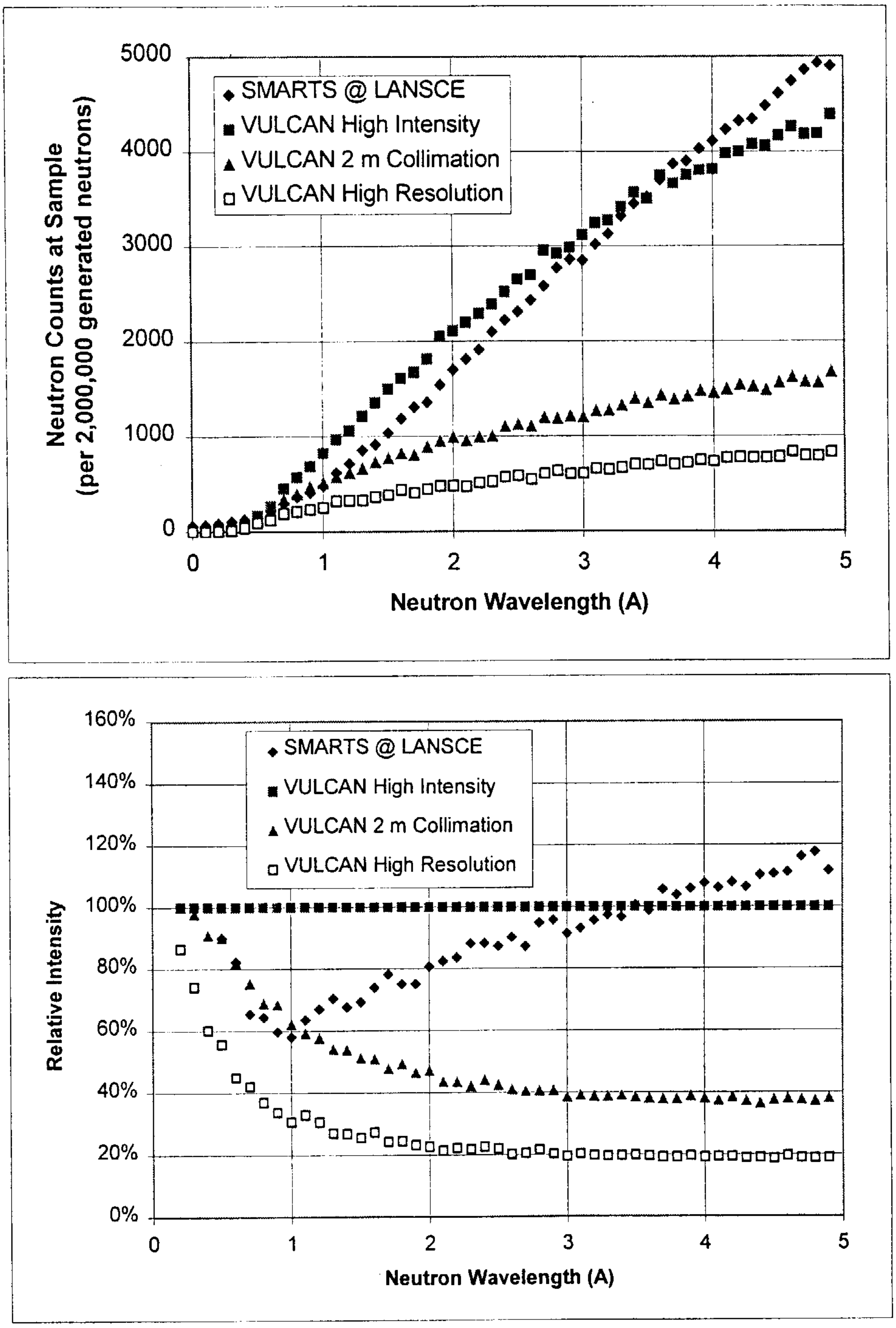

Fig. 9 Monte Carlo simulation to compare the performance of the neutron guide systems for SMARTS and VULCAN. Top panel: neutron counts at sample. Bottom panel: relative intensity with VULCAN high intensity mode as the baseline. The neutron source is a Lambert source with a uniform flux as a function of neutron wavelength. A 5×30 mm^2 sample is assumed. Choppers were not considered in either simulations. For comparison of actual flux, the neutron counts for VULCAN should be multiplied by a factor of 10 as the SNS source is 10 times more intense.

operating wavelength range of 0.8-3.0 Å, VULCAN shows a gain up to 60% in the high intensity mode. SMARTS has a slightly higher intensity at longer wavelengths (λ>3.3 Å). Note that for comparison of actual flux, the neutron counts obtained for VULCAN should be multiplied by a factor of 10 as the SNS source is 10 times more intense.

The performance gain for VULCAN's guide system is attributable to the use of $3\theta_c$ supermirror coatings on the sides. This is evident in Fig. 10, which compares the FWHM of the incident beam in the horizontal scattering plane. The region where VULCAN outperforms SMARTS is exactly where the FWHM shows a gain. It is interesting to note that the intensity for SMARTS varies linearly with λ^2, whereas the FWHM is proportional to λ for λ>0.4 Å. These kinds of dependence on λ are in fact characteristic of a long straight guide [4].

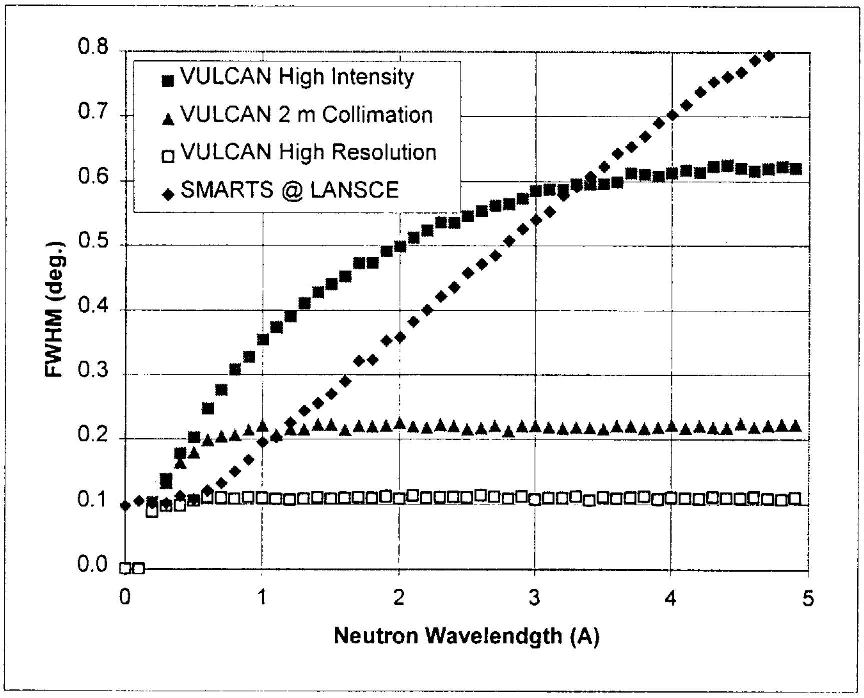

Fig. 10 Monte Carlo simulation results to compare the FWHM of the incident neutron beam in the horizontal scattering plane.

A question arising from Figs. 9-10 is whether this increased FWHM would spoil the resolution. To answer this question, the resolution function is compared in Fig. 7 for the 90° detectors (SMARTS is designed with one detector bank centered at 90°). As it can be seen, the resolution of VULCAN in the high intensity mode is comparable to that of SMARTS. Such a favorable comparison is due to careful optimization of the geometric contribution to the resolution function. By increasing the sample-detector distance from 1.5 m for SMARTS to 3 m for VULCAN, the contributions due to sample and detector sizes are greatly reduced. This has led to a geometric contribution (to the resolution function) comparable to that of SMARTS, despite the larger divergence of the incident neutron beam at the sample. Of course, VULCAN has much higher resolution in the 2 m collimation and high resolution modes.

Having established the baseline design, Monte Carlo simulation was then used to optimize the neutron guide system. While the optimization process is still in progress, some of the earlier results are presented below. Fig. 11 shows neutron intensity as a function of the starting position for the guide system. As it can be seen, there is no need to push the guide closer than 4 m from the moderator. This result significantly reduces the complexity of design work for the shutter. A parametric study of the bending curvature indicates that at the current value of 2 km, the bending radius of the curved guide is already optimized for suppressing the transmission of high-energy neutrons while allowing the maximum transmission for thermal neutrons with λ> 0.8 Å.

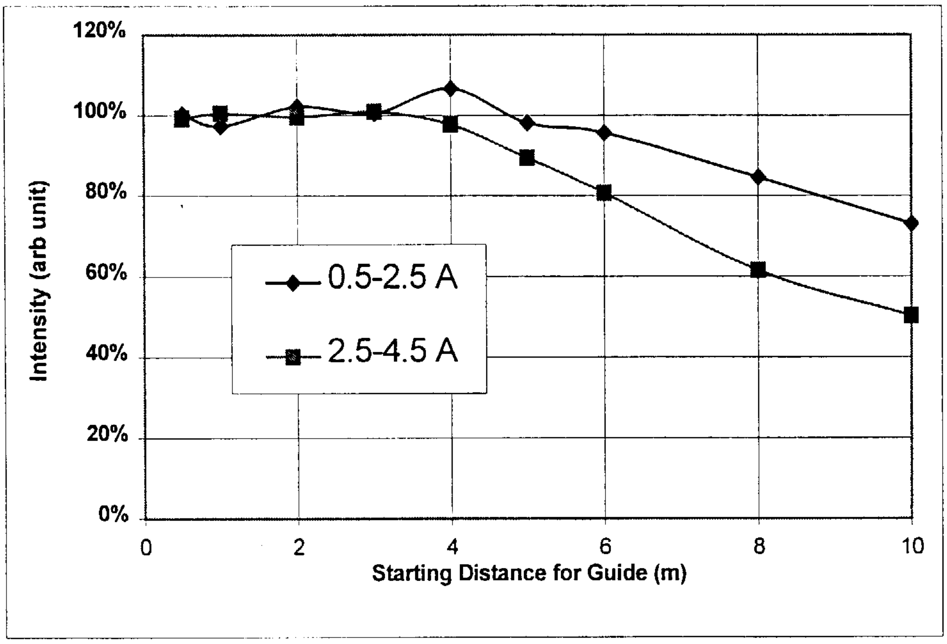

Fig. 11 Neutron intensity as a function of starting distance for the VULCAN guide system.

5. Summary

An effective neutron guide system has been proposed for VULCAN, the SNS engineering diffractometer. The proposed neutron guide system consolidates different performance requirements into one coherent design. Monte Carlo simulation confirms that the proposed neutron guide system is able to deliver the desired intensity and resolution. Parametric studies are underway with Monte Carlo simulation to further improve the performance of the neutron guide system.

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Acknowledgement

The authors wish to thank Dr. J. L. Robertson for his contribution in the development of IDEAS®. Oak Ridge National Laboratory is managed by UT-Battel, LLC, under contract DE-AC05-00OR22725 with the US Department of Energy.