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Spallation Neutron Source

Workshop Report

Workshop on the Design of the VULCAN Diffractometer

*held on March 7, 2001 at
Argonne National Laboratory*

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A U.S. Department of Energy Multilaboratory Project

SPALLATION NEUTRON SOURCE

Argonne National Laboratory • Brookhaven National Laboratory • Thomas Jefferson National Accelerator Facility • Lawrence Berkeley National Laboratory • Los Alamos National Laboratory • Oak Ridge National Laboratory

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Intense Pulsed Neutron Source
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Introduction

The design work for VULCAN, now the official title for the SNS engineering diffractometer, has progressed steadily. Continuing optimization using Monte Carlo simulation confirmed that the baseline design presented to the Instrument Oversight Committee was quite well optimized already. The simulation work did raise a question on the use of a multi-channel beam bender in lieu of a simple curved guide. A multi-channel beam bender shortens the distance at which high-energy neutrons become out-of-line-of-sight, thereby leading to substantial savings in shielding. However, the shortened flight path has implications on the resolution of the instrument which must be addressed. A reduced budget for neutron instrumentation at the SNS implies that all of the instruments need to be descoped. In light of this situation, the Instrument Advisory Team (IAT) must also decide on a basic functional instrument as well as an upgrade path. With the parameters for the neutron guide system reasonably well defined, it is time to consider the design of secondary components, such as the incident beam slit system, translators, and radial collimators. This workshop was intended for IAT members familiar with neutron instrumentation to discuss issues outlined above. The agenda of the workshop is provided in Appendix A and list of participants in Appendix B.

Design Progress with VULCAN

Xun-Li Wang reported the design status for VULCAN. Conceptual design for VULCAN was undertaken based on the desired performance determined by the user community [1]. The baseline design, schematically shown in Fig. 1, has been well documented [2] and approved by the Instrument Oversight Committee. The location for VULCAN has been changed from beamline #7 to #9. This move ensures that the entire instrument is housed within the target building, thereby eliminating the cost of constructing an extension to the target building which is about \$1-2M. Beamline #9 also provides easy access to the instrument, since there are no adjacent instruments to the right and it is close to a truck bay. Easy access is important for an instrument like VULCAN, since some of the specimens are of industrial-size and the ancillary equipment can be quite large as well. Fig. 2 shows a three-dimensional view of VULCAN at beamline #9.

Estimated performance for the baseline design is listed in Table I. In general, the estimated performance met the requirement by the user community. The Q-resolution ranges from 0.2% in the high resolution mode to 0.2-0.7% in the high intensity mode. It is worthwhile to note that the 0.2% resolution in the high resolution mode is consistent with the design goal of ENGIN-x at ISIS, UK [3] and POLDI at PSI, Switzerland [4].

For a 2MW source, the time-averaging neutron flux at the sample position was estimated to be between 10^7 and 10^8 $\text{cm}^{-2}\text{s}^{-1}$, depending on the mode of operation.

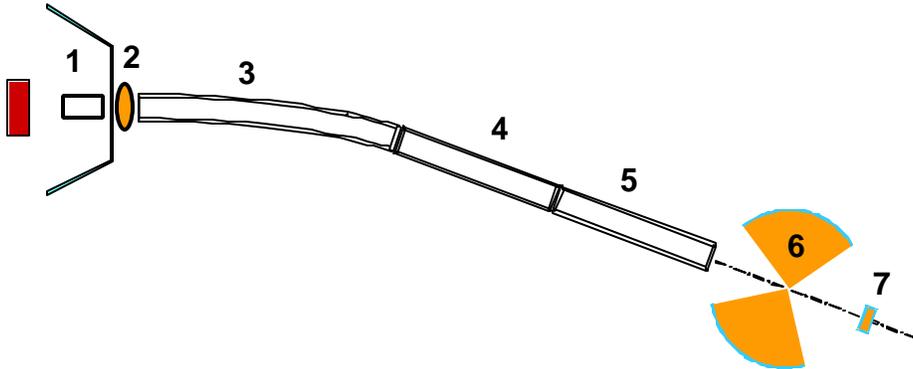


Fig. 1 Schematic of the base line design for VULCAN. The basic components and their characteristics are given below. All guides have a cross-section of 12×50 mm^2 and coated with 30_c supermirror on all sides

- 1 - in-monolith guide (3 m)
- 2 - band-width chopper
- 3 - curved guide (20 m, $R = 2$ km)
- 4 - straight guide (12 m)
- 5 - interchangeable unit (5 m)
- 6 - detector banks (60° - 150° in 2θ , $\pm 30^\circ$ in vertical plane)
- 7 - SANS detector (4 m from sample, 1 mm resolution)

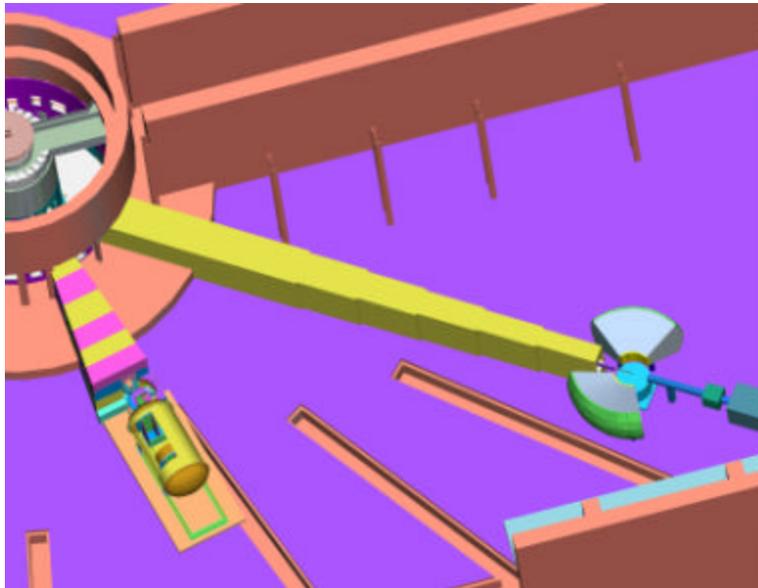


Fig. 2 A three-dimensional view of VULCAN at beamline #9

Table I. Estimated counting times for different types of experiments proposed for VULCAN.

Experiment Type	Desirable Parameters	Achievable Counting Time
3D mapping	1 mm ³	2 minutes
1D mapping	0.1 mm	60 min. (*)
In-situ Loading	~20 well separated peaks	1 min
Kinetic Measurements		0.1 sec
Diffraction & SANS	0.01-0.18 Å ⁻¹	sec
Bragg Edge (Transmission)		< 1 sec
(*) Estimated based on the Bragg Mirror technique [5], in which the entire depth profile is determined in one measurement.		

Monte Carlo simulation has been used to optimize the baseline design. The simulation work was carried out using IDEAS[®] (Instrument Design and Experiment Assessment Suite), a general-purpose software package developed at the Oak Ridge National Laboratory for simulating the optics of neutron scattering instruments [6]. Results obtained so far indicate that the baseline design was quite well optimized already. By varying the starting distance of the guide, it is shown that 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 confirms that at the current value of 2 km, the bending radius of the curved guide is optimized for suppressing the transmission of high-energy neutrons while allowing the maximum transmission for thermal neutrons with $\lambda > 0.8 \text{ \AA}$.

A simulation was carried out to investigate the possibility of replacing the curved guide with a multi-channel beam bender, which is essentially a curved guide with multiple reflective inserts. The advantage of a multi-channel beam bender as opposed to a simple curved guide is that the distance of out-of-line-of-sight can be substantially shorter. This will lead to significant savings in shielding cost. One outstanding issue associated with the use of a multi-channel beam bender is that the neutron intensity at the exit of the bender exhibits a severely uneven spatial distribution. Fortunately, Monte Carlo simulation results show that this uneven distribution is balanced by a 12-m straight guide following the beam bender. Monte Carlo simulations further show that for a multi-channel beam bender with n channels, the length of the bender may be shortened by a factor of n without changing the intensity or angular divergence of the neutron beam at the sample position, if the thickness of the reflective inserts is negligible. The shortened

beam path (by 10 m) does, however, have a negative impact the Q-resolution. In the high resolution mode, for example, the Q-resolution for the 90° detector bank deteriorates from 0.2% with a curved guide to 0.3% with a 2-channel beam bender.

Achieving 0.1 mm spatial resolution will be a challenge. Dr. A. D. Stoica, an expert in neutron optics, has been hired to develop the necessary technology that would enable this type of measurements.

Danny Williams gave an overview of the on-going engineering design. In particular, he discussed the design of the interchangeable guide-collimator system, which enables the instrument to operate flexibly for experiments having different intensity and resolution requirements. A highlight of his presentation was the animations which not only unveil details of each component but also show how the components are going to be assembled.

Design Considerations of Secondary Components

Translators

Specifications for the three-dimensional translator were discussed. Table II summarizes the design features of the translators in four instruments. Three of instruments are new, whose translators have a travel range of 300-600 mm for each axis. BT-8 at NIS is an existing instrument and has the smallest travel range. But Thomas Gnaeupel-Herold indicated that if given an opportunity to upgrade, he would like to double the travel range for all three axes. Mark Bourke emphasized the need for sufficient clearance from the sample table top to the beam height. A large clearance is needed in order to access to the area of interest in a large specimen. For SMARTS, the floor area where the sample table is located was recessed, leaving about 40-inch or 1-m maximum clearance from the top of the sample table to the beam height. The translator system for SMARTS was custom made by Advanced Design Consulting and costs about \$200 K. The BT8 translators were designed in-house by Paul Brand and has worked well. It features a relatively large mounting platform (380x600 mm²) with standard threaded holes. Walter Rimers of HMI liked the design and had requested a copy. The translators for the new NRSF instrument were custom made by Newport. It is a robust system with very high precision. For the ILL's new strain scanner, Phil Withers and Thilo Pirling are considering using hex-pods instead of regular translators. An advantage of the hex-pods is that individual legs can be moved independently, allowing the specimens to be tilted as well. However, the load capacity with hex-pods may be quite limited. A decision will be made fairly soon as to which approach would be used (hex-pods vs. regular translators)

Slits and radial collimators

For SMARTS, an automated slit system has been designed and will be used in the incident beam path. The outer dimension of the slit system is 200x200 mm². The width and height of the slit (made of boron nitride) are both continuously adjustable. The

diffracted beam will be defined using radial collimators. The slit system used in BT-8 is a commercial product made by Huber. Two neutron absorbing blades were tilted towards each other, forming a slit. The slit width is adjustable and the slit system can be positioned anywhere from 70 mm to 400 mm to the sample. The manual adjustable version costs \$3K, while the motorized version cost an additional \$2K.

Table II Comparison of the translator systems for selected instruments

	SMARTS* (LANL)	BT-8 (NIST)	NRSF* (ORNL)	ILL Strain Scanner*
X range (mm)	300	170	400	300
Y range (mm)	300	170	200	300
Z range (mm)	600	185	400	200
Precision (μm)	<100	Not specified	1	20
Load Capacity (kg)	1500	50	50	Light weight
Rotation	360°	360°	Upto 360° §	360°
* New instruments				
§ Depending on whether z-axis is mounted				

Radial collimators

Mark Bourke discussed the radial collimators for SMARTS. A set of ten radial collimators has been ordered, for a total cost of \$100K, to define a diffracted beam of various sizes. With the anticipated flux increase, spatial mapping with a sampling volume of $1 \times 1 \times 1 \text{ mm}^3$ is possible with SMARTS. In the highest resolution case, the radial collimator will need to be positioned at 10 cm to the sample position.

Mounting platform

Cam Hubbard presented a breadboard design for the mounting platform. The original idea was proposed by Peter Webster of Salford University (UK) during the VAMAS TWA-20 exercise. Breadboard platform with M6 tapered holes on 25 mm grid is an international standard for optical applications. To be compatible with the mounting platform, the base plates which hold the specimens should have matching 6 mm straight holes. With a common breadboard design, the specimen mounting procedures will be greatly simplified. Phil Withers suggested that in the future, each instrument should have multiple (e.g., 10) base-plates made. Users will be sent a base-plate prior to the experiments so that mounting of the specimens can be figured out at their home institutions. The standard breadboard design also enables easy transfer of a specimen between instruments. This will allow, for example, the measurement locations to be predetermined on an off-line alignment system using a coordination measurement machine (CMM). The breadboard mounting platforms are commercially available. Table III lists the TD series breadboard by Newport. Andy Winholtz commented that

Newport also makes a series of mounting devices and adapter for use on these breadboards.

Table III Specifications for the TD series breadboard by Newport.

Panel Thickness	1.08" (27.43 mm)
Surface Flatness	± 0.010 in. (.254 mm), over 2 ft (600 mm) square
Core Design	13/16" (20.6 mm) precision formed composite core (sealed hole tiles)
Sealed Mounting Holes	English 1/4-20 holes on 1 in. grid, 1.50 in. borders Metric M6-1.0 on 25 mm grid, 37.5 mm borders
Bottom Skin	10 GA (3.4 mm) steel
Weight	12 lbs./ft ²

Load frame and furnace

Ersan Unstundag described the load frame and the associated furnace attachment that he designed for SMARTS. Fig. 3 is a picture of the equipment which has been delivered to Los Alamos. At 950 kg, it is a very sturdy piece of equipment. The load force is 40,000 lb (or 180 kN) in static loading and 22,000 lb (or 100 kN) in dynamic testing. In terms of stress, these amount to a loading stress of 1.8 and 1 GPa, respectively, for a specimen with 1 cm² cross-section. The furnace attachment can be used standalone or with the load frame. The maximum temperature is 1500°C standalone or 1500°C with



Fig. 3 Load frame and furnace attachment for SMARTS

the load frame. There were four built-in windows for passing neutrons. The angular acceptance for these windows is $\pm 20^\circ$, adequate for making use of the out-of-plane detectors. Various sample environments are available, including vacuum and inert gas. Final tests at Los Alamos show that both the load frame and the furnace worked well. The cost for both items is \$500K.

Alignment system

SMARTS will use two theodolites for quick alignment of the specimen. Past experience at several facilities indicate that the precision with carefully calibrated theodolites is better than 0.1 mm. Phil Withers proposed using laser distancing devices. As an example, he mentioned a product made by Keyance which has an operating range of 750-150 mm with a precision of ± 20 micron. The cost in the UK is approximately £2500.

Software

Both SMARTS and NRSF will use LabView software by National Instrument for data acquisition and control. LabView was also the preferred choice for ENGIN-x, an upgraded instrument at ISIS. The custom made load-frame and furnace attachment for SMARTS was already controlled by LabVIEW, which should fit in well with the proposed data acquisition system. In terms of data analysis, Cev Noyan of IBM is taking the lead to develop an EXPERT system for analysis of the experimental data from SMARTS. In contrast to the Rietveld analysis approach currently used at ISIS, the EXPERT system will look at individual peaks recorded by each detector. The difference between these two approaches will become apparent when SMARTS started to generate data from real samples.

Discussions and Recommendations

The IAT members agreed that the baseline design for VULCAN met the performance requirement set forth by the user community. They also agreed that the estimated performance in terms of wavelength bandwidth, measurement speed, spatial resolution, and Q-resolution, was reasonable.

There were considerable concerns about the use of multi-channel beam benders. The IAT members were unanimously unwilling to accept the compromise to the Q-resolution resulting from the shortened beam path. They pointed out the importance of retaining a resolution of 0.2% for experiments needing high resolution. Thus, while the IAT members were happy to see a potential savings in the shielding cost, they were unwilling to give up the resolution.

Because detectors stand out as the single most expensive item for VULCAN, it is natural to consider the upgrade path by dividing the detectors into groups that will be installed in stages. As discussed in the conceptual design report [2], a fully equipped

VULCAN will have a wide detector coverage, from 60° to 150° in 2θ , and also a small angle area detector. However, the instrument will be functional, so long as detector banks at $\pm 90^\circ$ are furnished. Thus, a basic, functional VULCAN may well be the one with just 90° detector banks, much like SMARTS today and ENGIN-x as it is currently designed. Later, as more funds become available, the instrument can be upgraded to include high-angle detectors (upto 150°), low angle detectors (down to 60°), and the small angle detector.

Discussions were held on essential equipment that *must* be included in the basic, functional VULCAN. The list includes the following.

- A robust sample table with precision translators and a rotary stage. Data gathered in Table II suggests that each translator should have a travel range of 400-500 mm, a load capacity of 1500 kg, and a precision of no less than 100 μm for rough positioning and 10 μm for precise positioning.
- An automated and adjustable slit system for the incident beam path.
- A set of radial collimators for definition of the diffracted beam
- A coordination measurement machine for predetermination of the measurement coordinates. Phil Withers indicated that off-the-shelf commercial versions cost as low as \$40K.

It is important to note that the above list includes only the essential equipment that will make the instrument work. To produce high-quality scientific output, however, it is necessary to acquire a load frame and a furnace attachment similar to those designed for SMARTS. To produce unique sciences, VULCAN must be fully equipped with all detectors from 60° to 150° and the small angle area detector.

Phil Withers commented that past instrument efforts have mainly focused on hardware, while the development of software did not receive much attention. With several new instruments coming on-line in a few years, it is time to develop a comprehensive data analysis strategy and the needed software that will enable real-time data analysis. It would be particularly beneficial to the user community if the different groups could join hands and develop the analysis software together.

Tom Holden brought up the issue of expanding the user base in North America. On this topic, Phil Withers introduced the experience in Europe. In particular he mentioned the TRAINS program in the UK, which aims at attracting new users by bringing the novices to neutron scattering facilities and teaching them how to use the instruments. As a result of these outreaching efforts, Europe and the UK in particular have enjoyed a steady growth in new users. No such programs exist in the US or North America, except for a couple of generic workshops and summer schools which were launched only recently. It was generally agreed that a concerted outreaching effort should be started right away. Phil Withers suggested creating a periodic (e.g., semi-annual) newsletter, whose content may include introduction of instruments in North America neutron scattering facilities, and highlights of scientific and engineering research carried out at these facilities. Tom Holden agreed to serve as editor for such a newsletter. In addition, it was suggested that topical tutorial workshops should be held on a periodical basis.

Educational institutions such as the Joint Institute of Neutron Scattering and Oak Ridge Associated Universities are ideal vehicles for organizing these workshops.

Acknowledgement

I wish to acknowledge Ms. Carol Zimmer for her organization of the logistics and taking care of the myriad of details that ensured the workshop to proceed smoothly. Oak Ridge National Laboratory is managed by UT-Battell, LLC, under contract DE-AC05-00OR22725 with the US Department of Energy.

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5. A. D. Stoica, M. Popovich, and C. R. Hubbard, "Neutron Imaging with Bent Perfect Crystals. I. Imaging Conditions," *J. Appl. Cryst.*, **34**, 342-357 (2001)
6. X.-L. Wang and W.-T. Lee, "Monte Carlo Simulation of the Neutron Guide System for the SNS Engineering Diffractometer," pp. 513-524 in *Proceedings of ICANS-XV*, Vol. I, Japan Atomic Energy Research Institute, Japan (2001).

APPENDIX A Workshop Agenda

Wednesday, March 7, 2001

9:00 am	Objectives of the meeting	Xunli Wang
9:05 am	Design and estimated performance of VULCAN	Xunli Wang
9:45 am	Update on SMARTS	Mark Bourke
10:30 am	Break	
10:45 am	Translator system	Thomas Gnaeupel-Herold
11:15 am	Status of the SNS instrument suite	Kent Crawford
11:45 am	Sample mounting & alignment approach	Camden Hubbard
12:15 pm	Lunch	
1:30 pm	Load-frame & furnace attachment	Ersan Ustundag
2:00 pm	Update on ILL strain scanner	Phil Withers
2:30 pm	Long Wavelength Target Station	Jim Richardson (canceled)
3:00 pm	Break	
3:20 pm	Open discussions Is the design sensible (wavelength bandwidth, resolution etc.)? Any questions on the performance? What is a basic functional instrument? What are the upgrade paths?	
5:30 pm	Adjourn	

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