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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

Xun-Li Wang

Experimental Facilities Division
701 Scarboro Road
Oak Ridge, TN 37830

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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. This could lead 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 shown in Appendix A and a 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 summarized 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-averaged neutron flux at the sample position was estimated to be between 10^7 and 10^8 $cm^{-2}s^{-1}$, depending on the mode of operation.

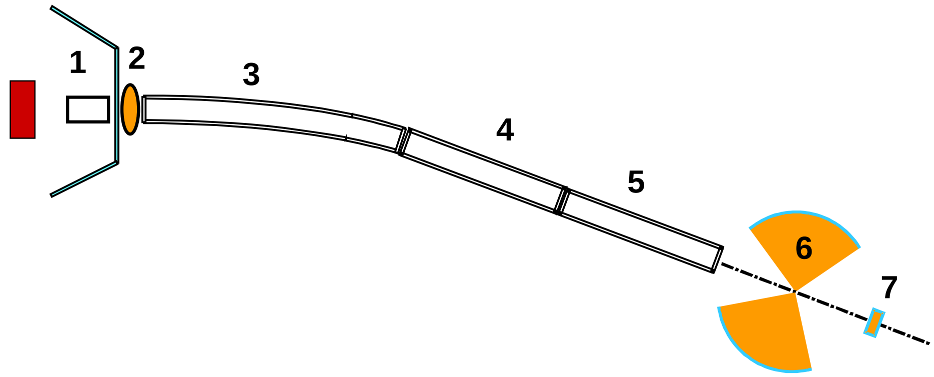

Fig. 1 Schematic of the base line design for VULCAN. The basic components and their characteristics are given below. All guides have a cross-section of 12x50 mm^2 and $3\theta_c$ supermirror coatings on all sides

1 - in-monolith guide (3 m)
2 - bandwidth 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, ±30° in vertical plane)
7 - SANS detector (4 m from sample, 1 mm resolution)

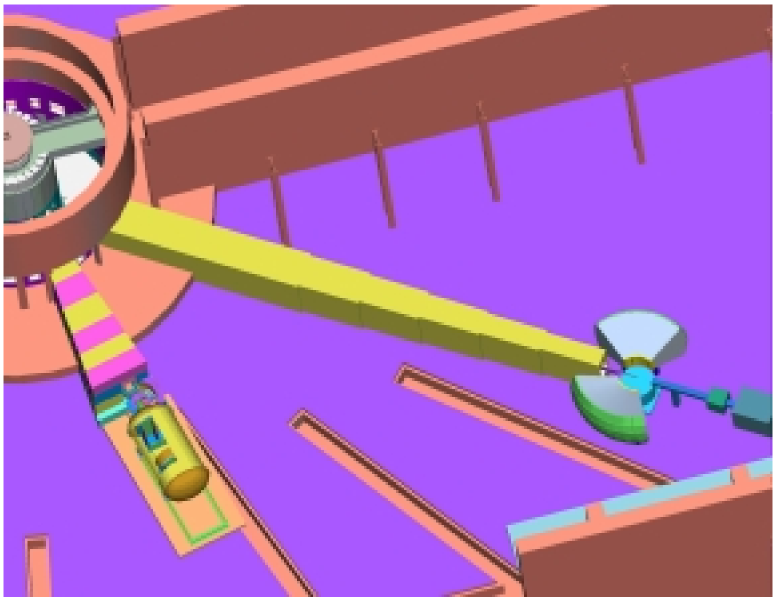

Fig. 2 A three-dimensional view of VULCAN at beamline #9

Table I. Estimated performance 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® (**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 [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 $\lambda > 0.8$ Å.

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 septa coated with reflective materials. 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 the 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, 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 septa 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 90º 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 update 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 showed not only the details of each component but also how the components are going to be assembled.

Design Considerations of Secondary Components

Translators

Specifications for the three-dimensional translator system were discussed. Table II summarizes the specifications for the translators of four instruments, three of which are new. For the new instruments, the translators have a travel range of 300-600 mm for each axis. The BT-8 at NIST is an existing instrument and has a travel range of 170-185 mm. But Thomas Gnaeupel-Herold, the instrument scientist of BT-8, 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 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 have worked well. It features a relatively large mounting platform (380x600 mm^2) 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

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 mm^2. 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 (at

NIST) is a commercial product made by Huber. Two neutron absorbing blades were titled 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	360º	360º	Upto 360º §	360º
* 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 1x1x1 mm^3 is possible with SMARTS. In the highest spatial resolution case, the radial collimator will need to be positioned as close as 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. If such a platform is adopted, 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 made by Newport. Andy Winholtz commented that Newport also makes a series of mounting devices and adapters 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

<u>Load frame and furnace</u>

Ersan Ustundag 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 60,000 lb (or 250 KN) in static loading and 22,000 lb (or 100 kN) in dynamic testing. For a specimen with 1 cm^2 cross-section, these amount to a loading stress of 2.5 and 1 GPa, respectively. The furnace attachment can be used standalone or with the load frame. The maximum temperature is 1800°C standalone or 1500°C with

Fig. 3 Load frame and furnace attachmnt for SMARTS

the load frame. There were four built-in windows for passing neutrons. The angular acceptance for these windows is ±20°, 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.

<u>Alignment system</u>

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.

<u>Software</u>

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. The EXPERT system will have both single-peak fitting and the Rietveld analysis codes. The users can choose either one to analyze the data.

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 ±90° 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 rotation 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 load frame and a furnace for in-situ time-resolved studies
- A coordination measurement machine for predetermination of the measurement coordinates. Phil Withers indicated that off-the-shelf commercial versions cost as low as $40K.

As indicated in [1], the real strength of VULCAN is time-resolved measurements at load and temperature. Thus, in order for the instrument to produce high-impact sciences, it is imperative to include the load-frame and furnace in the essential list of equipment. The full version of VULCAN should be equipped with all detectors from 60° to 150° and the small angle area detector and incorporate the technology for measurements with 0.1 mm spatial resolution. The fully equipped VULCAN will be able to produce unique sciences that no other instrument can.

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 well positioned to organize 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-Battel, 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	

APPENDIX B List of Workshop Participants

MARK BOURKE
Los Alamos National Laboratory
MS H805
Los Alamos, New Mexico 87545
phone: 505-665-1386
email: bourke@lanl.gov

KENT CRAWFORD
Argonne National Laboratory
IPNS Division, Bldg. 360
9700 South Cass Avenue
Argonne, Illinois 60439
phone: 630-252-7769
email: rkcrawford@anl.gov

ZHILI FENG
Engineering Mechanics Corporation of Columbus (EMC2)
3518 Riverside Drive, STE #202
Columbus, Ohio 43221-1735
phone: 614-459-3200
email: zfeng@columbus.rr.com

THOMAS GNAUPEL-HEROLD
National Institute Of Standards And Technology
100 Bureau Drive Stop 8562
Gaithersburg, Maryland 20899-8562
phone: 301-975-5380
email: thomas.gnaeupel-herold@nist.gov

DEAN R. HAEFFNER
Argonne National Laboratory
Bldg. 431
9700 South Cass Avenue
Argonne, Illinois 60439
phone: 630-252-0126
email: haeffner@aps.anl.gov

THOMAS HOLDEN
Los Alamos National Laboratory
MS H805 Lansce.DO
Los Alamos Neutron Science Center
Los Alamos, New Mexico 87545
phone: 505-665-3694
email: tmholden@lanl.gov

CAMDEN HUBBARD
Oak Ridge National Laboratory
PO Box 2008 MS6064
Oak Ridge, Tennessee 37831-6064
phone: 865-574-4472
email: hubbardcr@ornl.gov

BALASUBRAMANIAM RADHAKRISHNAN
Oak Ridge National Laboratory
PO Box 2008 MS6359
Oak Ridge, Tennessee 37831-6359
phone: 865-241-3861
email: radhakrishnb@ornl.gov
email: rad@mpm12.ms.ornl.gov

JAMES RICHARDSON
Argonne National Laboratory
IPNS Division, Bldg. 360
9700 South Cass Avenue
Argonne, Illinois 60439
phone: 630-252-3554
email: jwrichardson@anl.gov

A.D. STOICA
Oak Ridge National Laboratory
PO Box 2008 MS6430
Oak Ridge, Tennessee 37831-6430
phone: 865-241-0094
email: stoicaad@ornl.gov

ERSAN USTUNDAG
California Institute of Technology
Keck Engineering Laboratory
M/C 138-78
1200 E. California Blvd.
Pasadena, California 91125
phone: 626-395-2329
email: ersan@its.caltech.edu

XUNLI WANG
Oak Ridge National Laboratory
Spallation Neutron Source
Bldg. 7964H, room 110
MS 6430
Oak Ridge, Tennessee 37831
phone: 865-574-9164
email: wangxl@ornl.gov

DANNY WILLIAMS
Oak Ridge National Laboratory
Spallation Neutron Source
701 Scarboro Road
Oak Ridge, Tennessee 37830
phone: 865-574-9749
email: williamsdm@sns.gov

ROBERT (ANDY) WINHOLTZ
University of Missouri
Mechanical and Aerospace Engineering
Engineering Bldg. East, E2412
Columbia, Missouri 65211
phone:
email: winholtz@missouri.edu

PHILIP J. WITHERS
University of Manchester
Manchester Materials Science Center
Grosvenor St.
Manchester, M1 7HS, United Kingdom
phone: 44 161 200 8872
email: philip.withers@man.ac.uk