

PAPER • OPEN ACCESS

The TOSCA Spectrometer at ISIS: the Guide Upgrade and Beyond

To cite this article: R.S. Pinna *et al* 2018 *J. Phys.: Conf. Ser.* **1021** 012029

View the [article online](#) for updates and enhancements.

Related content

- [Cryogenic sample environment on TOSCA](#)
Richard B E Down, Anibal J Ramirez-Cuesta, Robert A Major et al.
- [Ionization of Helium by neutronic impact](#)
M J Ambrosio, D M Mitnik, G Gasaneo et al.
- [Proton drivers for neutrino beams and other high intensity applications](#)
R Garoby, K Gollwitzer, T Koseki et al.

The TOSCA Spectrometer at ISIS: the Guide Upgrade and Beyond

R.S. Pinna,^{1,2} M. Zanetti,^{1,2} S. Rudić,¹ S.F. Parker,¹ J. Armstrong,¹ S.P. Waller,¹ D. Zacek,¹ C. Smith,¹ S.M. Harrison,¹ G. Gorini,² and F. Fernandez-Alonso^{1,3}

¹ ISIS Facility, Rutherford Appleton Laboratory, Chilton, Didcot, Oxfordshire OX11 0QX, United Kingdom

² CNISM, Università degli Studi di Milano-Bicocca, Piazza della Scienza 3, 20126 Milano, Italy

³ Department of Physics and Astronomy, University College London, Gower Street, London WC1E 6BT, United Kingdom

E-mail: felix.fernandez-alonso@stfc.ac.uk

Abstract. We describe progress to date with the first major upgrade of the TOSCA spectrometer since it first became operational over fifteen years ago. This major project to boost the incident flux on the instrument by over an order of magnitude has been implemented in the past couple of years and has involved the complete redesign of the primary spectrometer to house a state-of-the-art, high-m neutron guide and associated chopper system. Engineering design and subsequent installation and commissioning efforts have been supported by extensive neutron-transport simulations and baseline studies of neutronic response in the context of the ISIS TS1 Project. Looking further ahead, we also outline ongoing feasibility studies to upgrade the secondary spectrometer, with a view to additional order-of-magnitude gains in neutronic and scientific performance.

1. Overview

The TOSCA instrument at the ISIS Pulsed Neutron and Muon Source is an indirect-geometry inelastic neutron spectrometer optimised for high-resolution vibrational spectroscopy in the energy-transfer range 0–4000 cm⁻¹ [1]. The instrument has been operational since the turn of this century and has become the gold standard for broadband chemical spectroscopy with neutrons [2–4]. As such, both TOSCA as well as its vibrant and growing science programme have been the inspiration for recent and exciting developments in novel neutron instrumentation across the globe. These include VISION at the SNS in the USA [5], LAGRANGE at the ILL in France [6], and VESPA at the ESS in Sweden [7]. Key factors to the success of TOSCA have been its high spectral resolution over a wide spectral range, its ease of use, as well as the full integration of contemporary computational materials modelling into its science programme. At present, its *INS Database* [8] contains over 700 entries, and these data continue to be mined by a growing community worldwide, in addition to fresh and exciting science on the instrument across materials chemistry, energy research and catalysis, to name a few areas of strength.

In 2013, an international panel of experts recognised the pressing need to boost the incident flux on the instrument, in order to move beyond the state-of-the-art in key scientific areas such as gas and charge storage [2, 3]. Following this exercise, extensive neutronic calculations have



been performed to benchmark the existing instrument in the context of the ISIS TS1 Project, as well as to provide a well-defined scientific and engineering specification. For further details, see Refs. [9–12]. These efforts have been followed by the construction and installation of the new guide over the past couple of years as well as by feasibility studies to upgrade the secondary spectrometer, as reported below.

2. The Guide Upgrade

The original geometry of the TOSCA primary spectrometer relied on simple (passive) collimation of the incident beam over a distance of 17 m. This configuration has served the instrument well over the past two decades, yet at the same time it did not capitalise on advances in neutron-guide technology for the effective delivery of neutron flux at the sample position. The first step in this project involved extensive Monte-Carlo simulations using the McStas package [13] to explore a suitable geometry for optimal neutron transport over a wide wavelength range without compromising the spectroscopic capabilities of the instrument. From these simulations, a tapered geometry with an increasing m -number over distance from the spallation target was chosen. These simulations predicted an average gain in flux well above one order-of-magnitude over the wavelength bandwidth of the instrument [2, 4, 10–12]. At the longest wavelengths accessible on TOSCA, these calculations indicated that gain factors could approach two orders of magnitude.

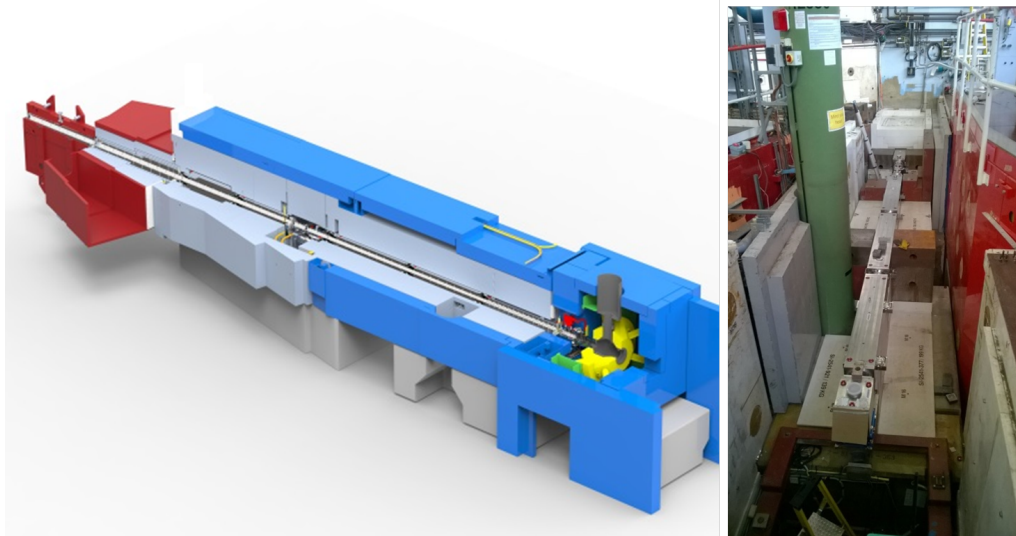


Figure 1. Left: Engineering design of the TOSCA guide following neutronics simulations. The ISIS TS1 target area is located on the left of the figure, whereas the TOSCA secondary spectrometer is depicted in yellow and green on the right-hand side. Right: Final stages of the first phase of the installation, completed in November 2016.

Figure 1 shows a schematic diagram of the engineering design of the guide according to the above specifications. Following manufacture by *Swiss Neutronics* over the period 2015-16, the guide was installed on TOSCA during the second half of 2016. In a first installation phase, all guide sections except the shutter insert inside the target monolith were installed, and this step was followed by a brief and preliminary commissioning period during December 2016. These two installation phases were required because of the radiation hazards associated with the handling of beamline components in close proximity to the spallation target. The preliminary commissioning tests that we have conducted during the first phase are very encouraging. The beam profile was found to be homogeneous across the sample area and the observed gains were somewhat higher

than expected from the neutronic simulations of the *baseline* scientific specification, particularly at long wavelengths. The second and final phase of the installation schedule was completed in the second half of February 2017 and has been followed by extensive commissioning tests on the instrument, due for completion at the end of March 2017. A detailed analysis of gains and other performance criteria is currently underway.

3. A New Secondary Spectrometer

TOSCA uses the (002) Bragg reflection from Highly Oriented Pyrolytic Graphite (HOPG) to effect final-energy selection. At present, each analyser bank on TOSCA consists of a flat square of area $\sim 144 \text{ cm}^2$, sitting at an average distance of 31 cm from the sample position. Its surface normal is placed at an angle of 45° relative to the scattered beam, leading to a final energy of *ca.* 28 cm^{-1} . A beryllium filter equipped with cadmium foils is placed between the HOPG analyser and the detectors to suppress higher-order HOPG reflections. This filter is cooled to *ca.* 30 K to improve the rejection of neutrons with energies above *ca.* 40 cm^{-1} . In its current incarnation, the HOPG analyser and the beryllium filter are very close to each other. While being a compact and practical solution requiring a relatively small HOPG analyser area, this feature also poses severe constraints on the overall neutron-collection efficiency of the secondary spectrometer.

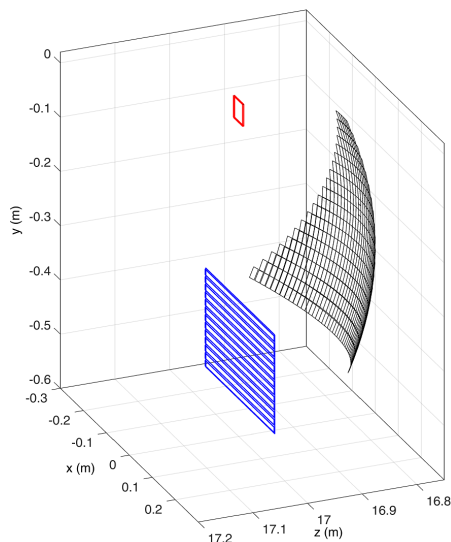


Figure 2. Curved HOPG analyser (black), sample (red), and detector array (blue).

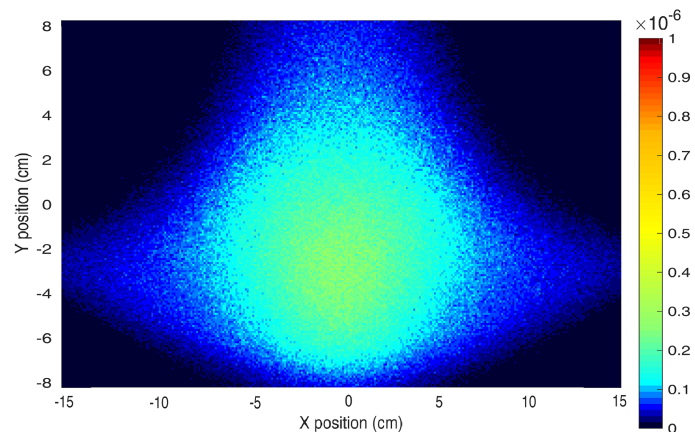


Figure 3. Spatial intensity distribution of detected neutrons from a parabolic HOPG analyser of total area 960 cm^2 .

To circumvent these limitations, we have started assessing other potential geometries that also build upon recent experience with similar instruments worldwide [5, 6]. Using the McStas package [13], we have created a custom component where HOPG tiles are arranged on either a spherical or parabolic surface of variable area. Figure 2 shows a three-dimensional view of the resulting computer model of a curved HOPG analyser, and Fig. 3 reports a typical spatial intensity distribution of detected neutrons. Preliminary Monte Carlo simulations and associated geometric optimisations using McStas [13] and iFit [14] have been performed as a function of analyser area and radius of curvature. These calculations show that an order-of-magnitude increase in detected flux is well within reach, particularly via the use of a parabolic (as opposed to spherical) analyser geometry. We have also found that the detected flux can be increased by optimising parameters such as the mosaicity of the HOPG array without compromising spectroscopic performance. In ideal circumstances, the surface of the curved HOPG analyser for

a given detector bank could be increased as much as to occupy an angular span of 60° , provided that engineering constraints can allow for it. Calculations have already been performed for three different sizes of doubly bent HOPG analysers of either spherical or parabolic shape. Our largest-area analysers amount to *ca.* 1500 cm^2 , a similar size to the one used earlier by Smee *et al.* at NIST to improve the performance of cold-neutron spectrometers [15, 16].

In a wider context, we note that the original conceptual design and subsequent scientific specification of TOSCA (and its predecessor TFXA) decades ago were solely performed on the basis of analytical calculations, a task that necessarily relied on a number of hard-to-test assumptions at the time. This situation is particularly true for the trade-off between flux and spectral resolution, as well as for the conditions required to attain an optimal match of the many different contributions to the neutronic response that are associated with both the primary and secondary spectrometers. The present work using modern neutron-transport codes, therefore, offers the exciting prospect of assessing in quantitative and unprecedented detail the relative importance of these parameters, including analyser shape and size, as well as time- and energy-focusing conditions. We, therefore, anticipate that the lessons learnt from this work will also have important implications for the optimal neutronic design of similar instrumentation in the foreseeable future.

Acknowledgements

The authors gratefully acknowledge the *Science & Technology Facilities Council* (STFC) for financial support for this project, including computing resources from the STFC Scientific Computing Department's SCARF cluster. This work has been partially supported by the 2014-2020 CNR-STFC Agreement concerning collaboration in scientific research at the ISIS Facility. We are also immensely grateful to *Swiss Neutronics* for the timely delivery of the guide components within specification.

References

- [1] WEB: www.isis.stfc.ac.uk/Pages/Tosca.aspx
- [2] Rudić S, Ramirez-Cuesta AJ, Parker SF, Fernandez-Alonso F, Pinna RS, Gorini G, Salzmann GC, McLain SE, and Skipper NT 2013 *Rutherford Appleton Laboratory Technical Report* RAL-TR-2013-015, Chilton. WEB: epubs.stfc.ac.uk/work/11216706
- [3] For a summary of the *TOSCA International Review* and its recommendations, see www.isis.stfc.ac.uk/Pages/TOSCA-Instrument-Review.aspx
- [4] Parker SF, Fernandez-Alonso F, Ramirez-Cuesta AJ, Tomkinson J, Rudić S, Pinna RS, Gorini G, and Fernández Castañón J 2014 *J. Phys. Conf. Ser.* **554** 012003.
- [5] Seeger PA, Daemen LL, and Larese JZ 2009 *Nucl. Instr. Meth. Phys. Res. A* **604** 719.
- [6] Jimenez-Ruiz M, Ivanov A, and Fuard S 2014 *J. Phys. Conf. Ser.* **549** 012004.
- [7] Fedrigo A, Colognesi D, Bertelsen M, Hartl M, Lefmann K, Deen PP, Strobl M, Grazzi F, and Zoppi M 2016 *Rev. Sci. Instrum.* **87** 0651014.
- [8] WEB: www.isis.stfc.ac.uk/Pages/INS-database.aspx
- [9] Pinna RS, Rudić S, Capstick MJ, McPhail DJ, Pooley DE, Howells GD, Gorini G, Fernandez-Alonso F 2017 *Nucl. Instr. Meth. Phys. Res. A* **870** 79.
- [10] Pinna RS, Rudić S, Parker SF, Gorini G, and Fernandez-Alonso F 2015 *EPJ Web of Conferences* **83** 03013.
- [11] Pinna RS, *MSc Thesis* (Università degli Studi di Milano-Bicocca, Italy, 2014). WEB: epubs.stfc.ac.uk/work/12257011
- [12] Fernández Castañón J 2013 *Rutherford Appleton Laboratory Technical Report* RAL-TR-2013-002, Chilton. WEB: epubs.stfc.ac.uk/work/65395
- [13] Willendrup PK, Udby L, Knudsen E, Farhi E, and Lefmann K 2011 *Nucl. Instr. Meth. Phys. Res. A* **634** S150. WEB: www.mcstas.org
- [14] Farhi E, Debab Y, and Willendrup P 2014 *J. Neut. Res.* **17** 5.
- [15] Smee SA, Orndorff JD, Scharfstein GA, Qiu Y, Brand PC, Broholm CL, and Anand DK 2002 *Appl. Phys. A* **74** S255.
- [16] Smee SA, Brand PC, Barry DD, Broholm CL, and Anand DK 2001 *Nucl. Instr. Meth. Phys. Res. A* **466** 513.