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Detailed characterisation of the incident neutron beam on the TOSCA spectrometer

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Figures: 7

Tables: 1

Abstract

We report a detailed characterisation of the incident neutron beam on the TOSCA spectrometer. A bespoke time-of-flight neutron monitor has been designed, constructed and used to perform extensive spatially resolved measurements of the absolute neutron flux and its underlying time structure at the instrument sample position. The obtained data give a quantitative understanding of the current instrument beyond neutronic simulations and provide a baseline in order to assess the performance of the upgraded instrument. At an average proton current-on-target of 153 μA (ISIS Target Station 1; at the time of measurements) we have found that the wavelength-integrated neutron flux (from 0.28 Å to 4.65 Å) at the position of the TOSCA instrument sample (spatially averaged across the 3 x 3 cm^2 surface centred around (0,0) position) is approximately 1.2 x 10^6 neutrons cm^{-2} s^{-1}, while the whole beam has a homogeneous distribution across the 3.0 x 3.5 cm^2 sample surface. The spectra reproduced the well-known shape of the neutrons moderated by the room temperature water moderator and exhibit a neutron flux of 7.3 x 10^5 neutrons cm^{-2} s^{-1} $Å^{-1}$ at 1 Å.

Keywords: TOSCA, neutron beam profile, neutron detector, scintillator detector, neutron flux

1. Introduction

TOSCA [1] is a world leading inelastic neutron spectrometer that has set the standard for broadband vibrational spectroscopy with neutrons. The instrument is characterised by its 17 m primary flightpath and 4.0 x 4.0 cm^2 beam size at the sample position [2].

For the instrument to keep pace with the scientific challenges, an increase in the neutron flux collected at the sample position through a supermirror neutron guide placed along its beamline, would be highly beneficial. Such neutron beam should remain well focussed and its neutron flux should be uniform. In order to evaluate the beam features we have designed and built a detector assembly that conforms to the space constraints of the TOSCA instrument, and allows us to characterise the neutron beam profile. Therefore here we present the time-of-flight (TOF) measurements performed at different points along the TOSCA sample position surface. These results are of utmost importance in defining the current instrument baseline and for the assessment of the performance gain that will be achieved after the installation of the neutron guide along the TOSCA beamline [3,4,5].

TOSCA views a 300 K water moderator placed upstream of the North 8 beamline (TOSCA) at ISIS Target Station 1. The moderator is 120 mm high, 125 mm wide and 45 mm deep and it has a gadolinium poisoning foil placed at a distance of 15 mm from the north face of the moderator [6]. The water vessel is surrounded by a beryllium neutron reflector and by an in-reflector borated decoupler that reduces the pulse time-width.

2. Experimental setup

ISIS Facility is a pulsed neutron and muon source with a frequency of 50 Hz, i.e. the period between the pulses is 20 ms (a sub-frame) and the pulses are arranged in frames with duration of 100 ms. TOSCA receives 4 pulses in a single frame while the last pulse of the source is redirected towards the second target station, see Figure 1. The missing pulse is exploited to extend the energy transfer range of the instrument at a relatively small cost as this high TOF region contains the intense elastic line. This mode of operation has proved valuable and was recently adopted on VESUVIO instrument at ISIS to extend its energy range down to 1 meV quite successfully [7].

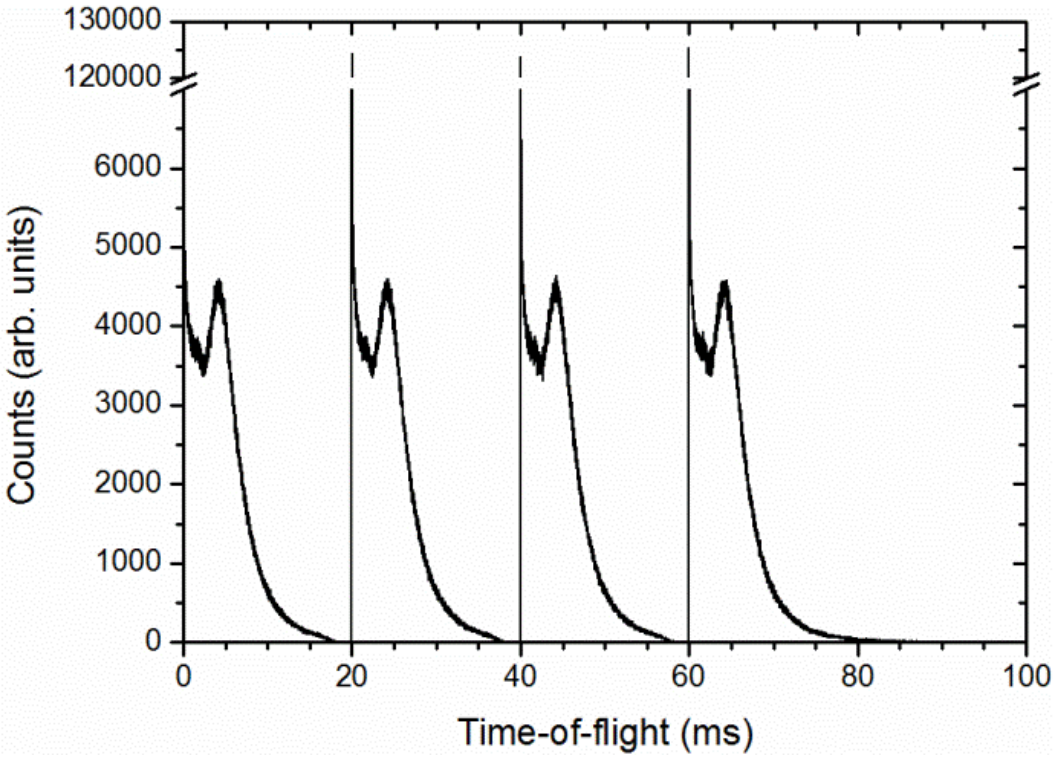

Figure 1. Time-of-flight spectra of neutrons within the single TS1 frame recorded with the help of a GS1 detector at the TOSCA sample position.

The beam profile was probed using a calibrated neutron beam monitor/detector designed to measure the neutron flux. The sensitive component of the detector is a cuboid of cerium-doped glass scintillator, measuring 0.96 x 0.95 x 0.53 mm^3. The scintillator known as 'GS1' (purchased from Scintacor, formerly known as Applied Scintillation Technologies) contains 2.4% lithium by weight with natural isotopic abundance and was sized to provide a point-like sample of the neutron beam, removing the possibility of edge-effects or misalignment affecting the data. The GS1 scintillator was enclosed within the aluminium detector housing, and mounted via an aluminium shaft on a set of XY motorized translational stages, see Figure 2. The whole assembly was set on the 180 mm diameter flange (499 mm above the beam axis) that gives direct access on top of the sample position. The choice of the lower flange as the main support has been made to reduce the length of the translational shaft, thus reducing the likelihood of misalignments. The TOSCA closed cycle refrigerator (CCR) needed to be removed from its position in order to accommodate the assembly frame onto the flange, and thus the measurements at the sample position were performed in open air and at room temperature.

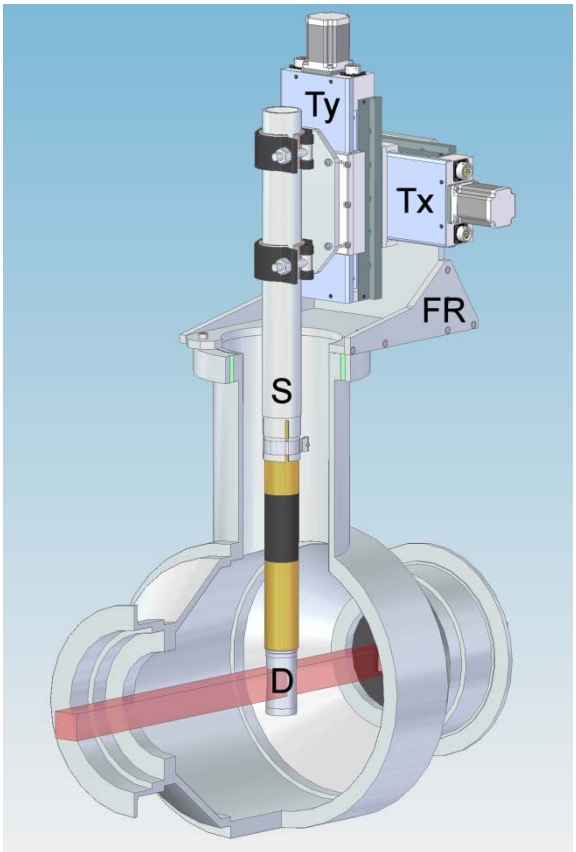

Figure 2. The experimental setup for measuring the neutron beam profile on TOSCA instrument. It includes a GS1 detector (D) enclosed within the aluminium housing, and mounted via an aluminium shaft (S) on a set of XY motorized translational stages (Tx, Ty). The assembly frame (FR) was positioned in such a way for the detector to overlap with the beam path denoted in pink.

The position of this point-sampling detector was controlled via a computer script which moved it automatically after the accumulation of 20000 frames at each spatial point (1 frame = 100 ms), each frame containing four consecutive neutron pulses, without the need to interrupt the beam between different runs. Over 100 points around the beam centre (from -3.0 cm to +3.0 cm in the X (horizontal) and Y (vertical) directions, when looking downstream) were measured, sampling the time-of-flight spectrum across the beam cross section almost every 5 mm, see Figure S1 in supplementary information (SI). Subsequently the data were calibrated to give the neutron flux at the sample position in units of neutrons cm^{-2} s^{-1} $Å^{-1}$ and eventually integrated in the wavelength range of interest.

It is worthwhile to point out that the TOSCA beamline is composed of the shutter tube, a monolith tube and five subsequent collimation tubes, where each section contains various

collimation inserts (B4C neutron absorbing rings) and sections (all tapered) are separated by the thin aluminium windows to preserve the vacuum. See reference 2 for precise details. At the time of this study only the monolith tube and two subsequent collimation tubes were under vacuum.

Computational details: The McStas software package [8] was used in order to perform Monte Carlo simulations of the neutron scattering at the TOSCA beamline. The geometrical parameters of the instrument primary beamline [4] were implemented in the virtual instrument, while the water moderator file [9] was provided by the ISIS Neutronics Group and was built using MCNP-X calculations of the actual TS1 target-reflector-moderator assembly. The angle between the TOSCA beamline axis and the moderator face was kept at 90º i.e. the moderator face and the shutter face were perfectly aligned/parallel. In reality the beamline axis is tilted by ~13.2º from the line perpendicular to the moderator face and this information has been taken into account when generating the moderator file. Thus for the purposes of McStas calculations the difference between the real and the simulated angle is not important.

3. Methodology of data analysis

The Mantid software package [10,11,12] was used in order to analyse the time-of-flight spectra recorded with the help of the GS1 detector at various points across the sample surface. Each spectrum covered the region between 0 and 100 ms (one frame), it was composed of five sub-frames, and the data bin had constant width of 4 μs across the whole spectrum. The spectrum signal to noise ratio was improved by accumulating 20000 frames at each spatial point.

The data processing consisted of the following steps:

(a) The retrieved raw TOF data in the range from 0 to 100 ms were separated into five equal parts of 20 ms each i.e. the four TS1 pulses plus the TS2 pulse. The last part (sub-frame) is not influenced by the TOSCA neutron beam chopper and allows the study of the TOSCA elastic region around 3.4 meV i.e. ~22 ms from the start of the neutron pulse [2], which is

normally shadowed by the frame overlap, as shown in Figure 1 and described in the previous section.

(b) The first four sub-frames were summed into one single histogram and the resulting TOF spectrum was converted into a wavelength spectrum. This is a linear conversion of TOF units which at length of 17 m from the moderator corresponds to the following equation:

$$\lambda[\text{Å}] = \frac{h}{m}\frac{t}{L} = 2.327 \times 10^{-1} t[ms] \quad (1)$$

where h = 6.63x10^{-34} Js is Planck's constant and m is the neutron mass. Although the total number of data bins upon transformation stays the same their width is shrunk; furthermore the data values of the intensity (counts) were not adjusted or rearranged as a result of the conversion.

(c) In order to derive the real number of neutrons in each wavelength bin N_{eff} the measured counts C needed to be corrected by the wavelength dependent efficiency ε(λ) of the current (GS1) detector:

$$N_{eff}(\lambda) = \frac{C}{\varepsilon(\lambda)} \quad (2)$$

where ε(λ) can be calculated using the properties in Table 1.

$$\varepsilon(\lambda) = 1 - e^{-N\sigma(\lambda)l} \quad (3)$$

Table 1. Physical properties of GS1 scintillator detector containing lithium.

Physical property	GS1 detector
area [m^2]	9.12 x 10^{-7}
density [kg m^{-3}]	2.66 x 10^3
mass fraction of Li_2O within detector	6.00 x 10^{-2}
mass fraction of Li within Li_2O	4.64 x 10^{-1}
isotopic abundance of ^{6}Li	7.60 x 10^{-2}

molecular weight of ^{6}Li [kg mol^{-1}]	6.00 x 10^{-3}
number of moles of ^{6}Li [mol m^{-3}]	9.38 x 10^{2}
Avogadro constant [mol^{-1}]	6.02 x 10^{23}
N of ^{6}Li [atoms m^{-3}]	5.65 x 10^{26}
^{6}Li σ_{abs} at 1 Å [m^{2}]	5.22 x 10^{-26}
thickness *l* [m]	5.30 x 10^{-4}
Nσl (at 1 Å)	1.56 x 10^{-2}

In the linear approximation for the wavelength dependence of the lithium absorption cross section [13], equation (2) reduces to:

$$\varepsilon(\lambda) = 1 - e^{-Al\lambda} \tag{4}$$

where $A = N\sigma_{abs}(1\text{Å})$ is the absorption coefficient [Å^{-1}m^{-1}], l is the detector thickness [m] and λ is the neutron wavelength [Å]. For the GS1 detector A = 29.49 Å^{-1}m^{-1} and l = 0.53 mm.

Subsequently N_{eff} was normalized by the detector area of 9.1 x 10^{-3} cm^{2} in order to derive the number of neutrons per unit area, and divided by the total number of summed frames (i.e. 20000 frames). Considering that TOSCA receives 10 frames per second, scaling the results by that factor (10) eventually gives the spectrum of the time averaged neutron flux on the sample in units of neutrons cm^{-2} s^{-1} as a function of wavelength. Furthermore, if one takes into account the normalisation by the wavelength bin size (i.e. 9.3 x 10^{-4} Å) one can get the neutron flux intensity in units of neutrons cm^{-2} s^{-1}Å^{-1}. Finally, we integrated this final spectrum across the wavelength range which is relevant for TOSCA (i.e. from 0.28 Å to 4.65 Å) to get the total useful neutron flux that impinges on the sample during a second.

5. Results and discussion

The experimentally derived TOF spectrum as a function of wavelength of the TOSCA neutron flux (spatially averaged across the 3.0 x 3.0 cm^{2} surface centred around (0,0) position) is shown in Figure 3 (black trace). Its features are in line with the expectations [14] since the peak in the 'moderated hump' appears at around 1 Å which is characteristic of room temperature water moderator. Its shape is characterised by the epithermal component at low

wavelength and the Maxwellian component that follows. Equally, in terms of its overall profile the experimental spectrum is in line with the results of the Monte Carlo simulations (red empty triangle symbols) performed with the help of McStas software, although the latter needed to be scaled down by the factor of 3.41 in order to make the simulated and the experimental integrated neutron flux in the region between 0.28 Å and 4.65 Å equal. Furthermore, it is comparable in shape to the POLARIS (ISIS diffractometer located next to TOSCA instrument) spectrum while the fluxes have the same order of magnitude [15]. This is not surprising since both instruments share the same moderator, and the higher flux on POLARIS is mainly due to its shorter beamline (14.0 m). The TOSCA beam profile at the sample position is shown in Figure 4.

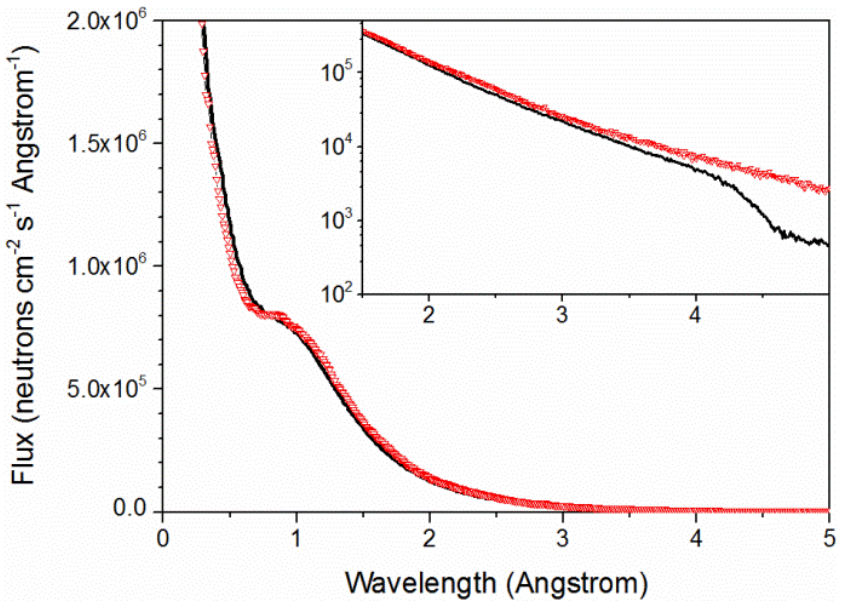

Figure 3. Neutron flux at the TOSCA sample position as a function of wavelength. Experimentally derived values (spatially averaged across the 3.0 x 3.0 cm^2 surface centred around (0,0) position) are shown as black line while those obtained with the help of Monte Carlo simulations are shown in red as empty triangle symbols. Monte Carlo values of the neutron flux were scaled down by the factor of 3.41 in order to make the simulated and the experimental integrated neutron flux in the region between 0.28 Å and 4.65 Å equal. In order to make easier comparison at the higher wavelengths, the inset (in the upper right corner) shows the neutron flux (in logarithmic scale) as a function of wavelength. The drop in the experimental flux for neutrons with the wavelength larger than 4 Å is a consequence of the disc chopper used to prevent the frame overlap [2].

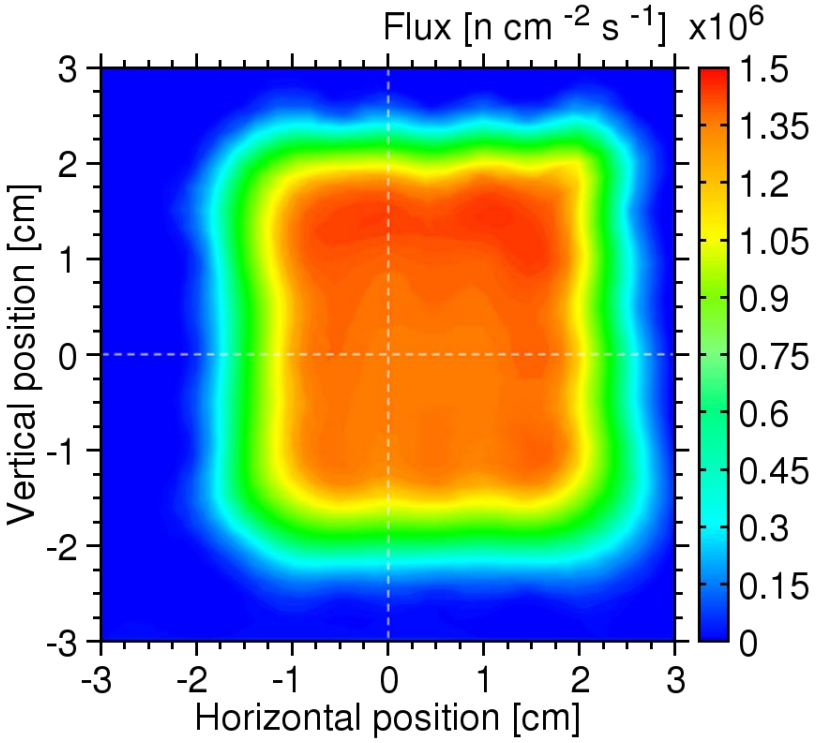

Figure 4. The experimentally derived neutron beam profile at the TOSCA sample position. The measured values of time averaged neutron flux, integrated across 0.28 Å to 4.65 Å wavelength range of interest to TOSCA, were obtained with the average proton current-on-target of 153 μA.

Its central region, 2.0 x 2.0 cm^2 in area, is homogeneous, while overall beam has roughly 3.8 (H) x 4.0 (V) cm^2 square shape (taking into account the region with the neutron flux higher than 50% of the maximum intensity) as a consequence of the long collimator positioned along the beamline. In the upper right section of the beam profile higher neutron flux can be observed, while the beam centre appears to be displaced (up and to the right when looking downstream, i.e. from the moderator towards the instrument). Such hotspot could be due to the non-uniformity of the beam exiting the moderator face. It is less pronounced if one looks into the higher wavelength neutrons that spend longer period of time in the moderator, making more collisions in the water and thus have more chance to distribute evenly across the moderator surface. The evaluation of the beam spatial profile as a function of wavelength is shown in Figure 5. In particular, the beam profile for neutrons with the wavelength between 0.8 Å and 1.2 Å has higher flux in the upper right corner, while the beam profile for neutrons with the wavelength between 2.5 Å and 2.9 Å is much more uniform across the

whole beam surface. The beam shift may indicate shutter misalignment, possible unwanted reflections or simply displacement of the instrument centre from the beamline axis.

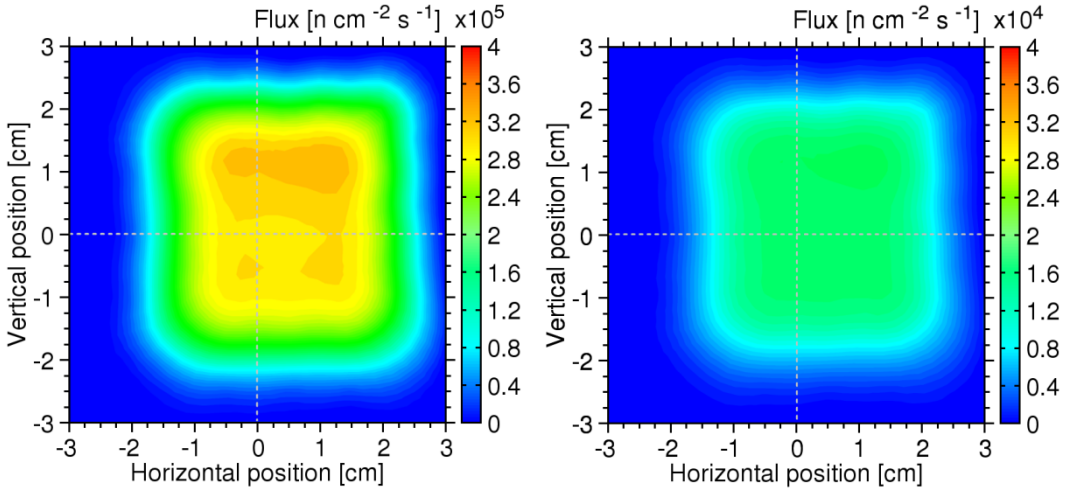

Figure 5. The experimentally derived neutron beam profiles at the TOSCA sample position for neutrons with the wavelength between 0.8 Å and 1.2 Å (left) and 2.5 Å and 2.9 Å (right). The measured values of the time averaged neutron flux were obtained with the average proton current-on-target of 153 μA. Note that the two scales differ by the order of magnitude.

The theoretical simulation of the TOSCA beam profile at the sample position is depicted in Figure 6. The simulated beam has roughly 4.8 (H) x 4.8 (V) cm^2 (taking into account the region with the neutron flux higher than 50% of the maximum intensity) square profile (due to the collimation), while the flux is constant across the 4.0 (H) x 4.0 (V) cm^2 surface as further indicated by the horizontal cross cut across the beam intensity, see Figure 7. As emphasized before the simulated neutron flux is 3.41 times higher than the experimentally observed values. This is not surprising since the simulation was performed in vacuum while in reality, at the time of this experiment out of a 17 m long flightpath between the moderator face and the TOSCA sample position, only 7 meters were under vacuum and 10 meters were in air. Thus in order to compare with the experiment, the simulated values should be corrected by the factor of 0.52 which corresponds to the transmitted neutron flux upon travel through 10 m of air. The corrected simulated values are shown in Figure 7 as well. They are still 1.77 (3.41 x 0.52) times larger than the experimental values, and the difference can be ascribed to various factors. Namely, the simulation does not take into account the aluminium windows positioned along the primary flightpath, and the expected differences between the

full neutronics simulation of the neutron production in the TS1 target-reflector-moderator assembly and the experimental neutron flux [16].

Figure 7 points to the neutron beam that is somewhat shifted from the beam centre to the right. Furthermore, it is apparent that the experimental beam width is smaller than predicted. The plateau of the simulated profile is exactly 4.0 cm in width while the experimentally observed width has a plateau of about 3.0 cm. As one can see from the Figures 4 and 6, the measured and the calculated neutron flux at the centre of the sample, at the so called (0,0) position (see SI), are 1.3 x 10^6 neutrons cm^{-2} s^{-1} and 4.1 x 10^6 neutrons cm^{-2} s^{-1}, respectively. The corresponding values spatially averaged across the 3.0 x 3.0 cm^2 surface centred around (0,0) position are 1.2 x 10^6 neutrons cm^{-2} s^{-1} and 4.1 x 10^6 neutrons cm^{-2} s^{-1}, respectively. Between the two later values a normalization factor of 3.41 might be applied to match the absolute values. The neutron flux values associated with the plateau shown in Figure 7, and averaged along the vertical axis (between -2.0 cm and +2.0 cm) are slightly smaller. In particular the simulated values were derived with the help of the linear flux monitor, i.e. not the wavelength monitor used in the case of the beam profile shown in Figure 6.

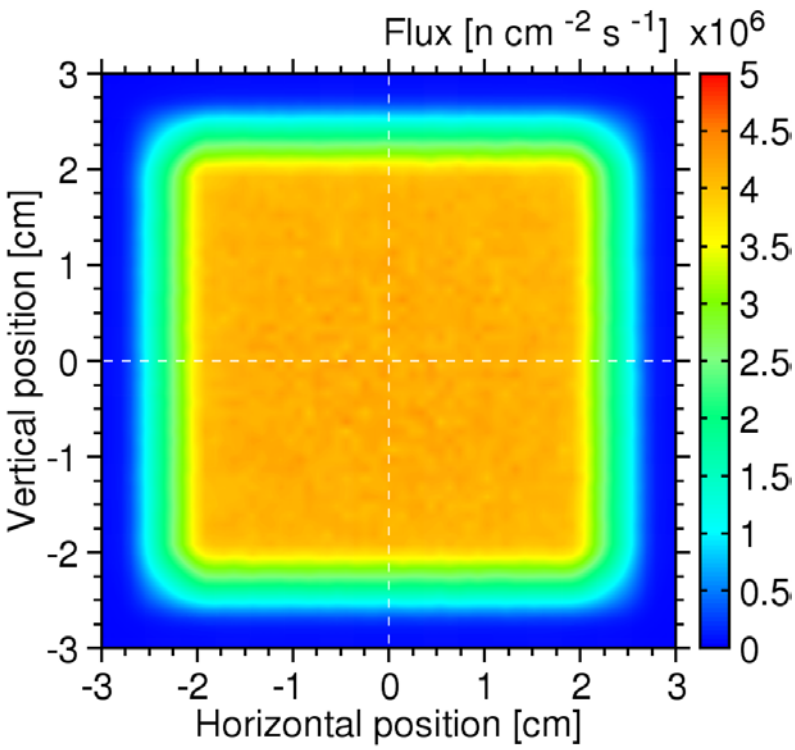

Figure 6. The simulated neutron beam profile at the TOSCA sample position. The calculated values of the time averaged neutron flux, integrated across 0.28 Å

to 4.65 Å wavelength range of interest to TOSCA and scaled to the averaged proton current-on-target of 153 μA.

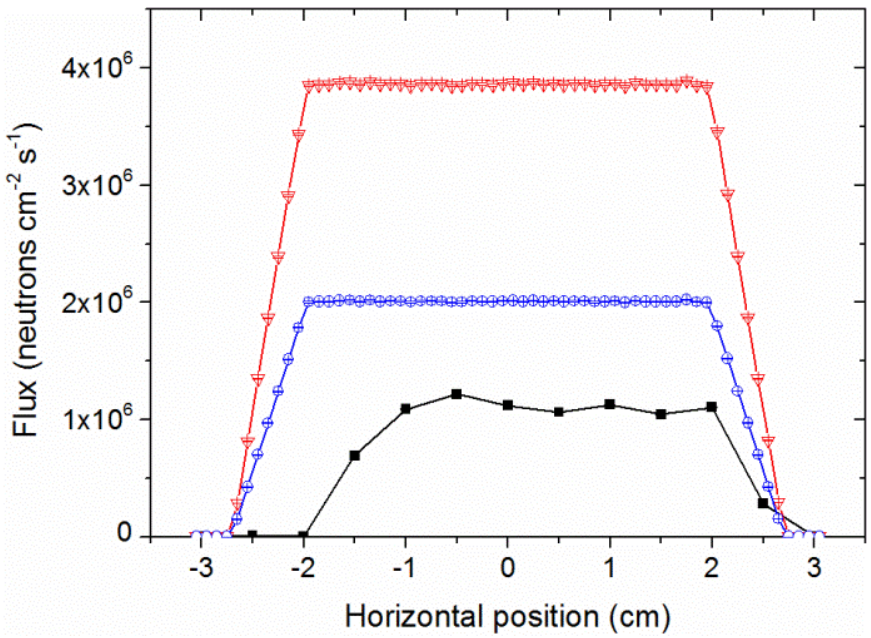

Figure 7. The experimental (black filled squares), the simulated (red empty triangles) and the corrected simulated (for attenuation in air; blue empty circles) neutron beam profile projected along the horizontal axis at the TOSCA sample position. The beam flux has been averaged along the vertical axis (between -2.0 cm and +2.0 cm, i.e. within the beam height) and includes only neutrons within the wavelength range of interest to TOSCA (from 0.28 Å to 4.65 Å).

Conclusions

The results evidenced that the incident beam on TOSCA has a strongly collimated square shape, with a steep fall in intensity outside the main region. The penumbra of the beam is a 0.5 cm crown around the main beam spot at its broadest size on the bottom. The beam appears reasonably homogeneous across the 3.0 (H) x 3.5 (V) cm^2 surface, although some beam patterns can be observed, and the illuminated area is approximately 3.8 (H) x 4.0 (V) cm^2. The time averaged wavelength-integrated flux at the TOSCA sample centre, so called (0,0) position, is around 1.3 x 10^6 neutrons cm^{-2} s^{-1} and we measured the flux of 7.3 x 10^5 neutrons cm^{-2} s^{-1} Å^{-1} at the moderator peak (~1 Å) which represents the Maxwellian component of the incident spectrum. The measurements reveal the neutron beam profile that is ~35% smaller (by area), and the neutron flux in the beam centre (spatially averaged across

the 3.0 x 3.0 cm^2 surface centred around (0,0) position) that is 3.41 (1.77, after correction for attenuation in air) times smaller than predicted by the Monte Carlo calculations.

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Supplementary Information
for
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Procedure used in order to generate the image of the neutron beam profile in Figures 4 and 5.

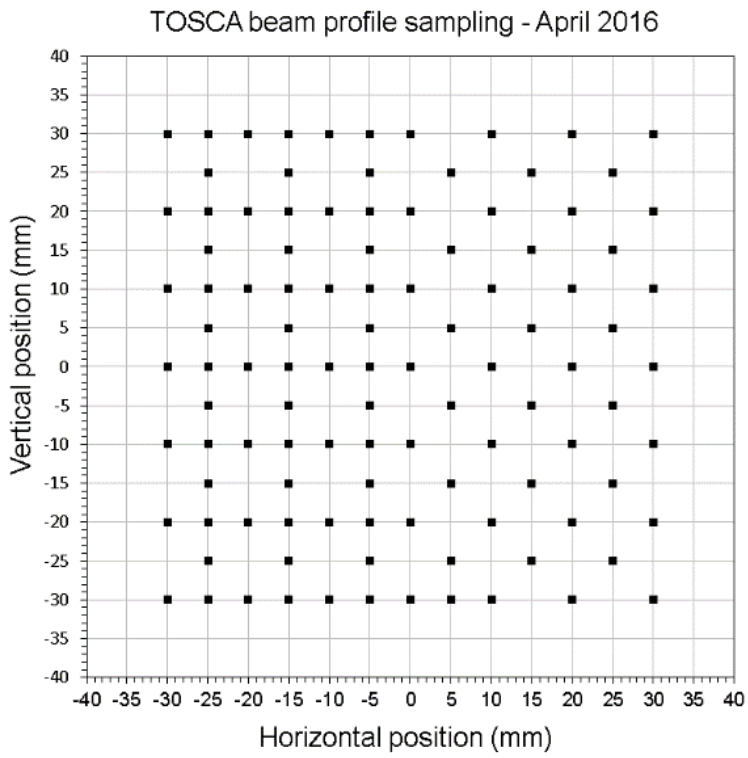

Figure S1. Map of the positions across the TOSCA sample surface (around the beam centre, and when looking downstream, i.e. from the moderator towards the instrument) where the neutron flux has been measured.

The data from each sampling point shown in Figure S1 was retrieved as a TOF spectrum and reduced by means of the procedure described in the main text of the article. From the data analysis we could obtain the wavelength spectrum in units of neutron cm^{-2} s^{-1} $Å^{-1}$ which was integrated from 0.28 to 4.65 Å to get the operationally useful neutron flux for TOSCA at each point. The flux value was associated with the corresponding X-Y coordinate of the sampling point across the sample surface; we could then derive a three column array (X-Y-Flux) that could be plotted in Origin (Data analysis and Graphing Software) as a contour plot, where the colour scale is linked to the flux magnitude. Furthermore, since the sampling step between the points is not uniform across the surface we smoothed the picture by averaging values between the data points.

Procedure used in order to derive the 1D neutron flux curve (see Figure 7).

To obtain the neutron flux curve in 1D, namely along the horizontal axis along the sample median line, we selected all the experimental points placed at the same horizontal position (see Figure S1), converted to units of flux and then averaged the values along the vertical axis from -2.0 cm to +2.0 cm. Finally we generated the plot of the average flux values across the sample as a function of the horizontal position.

To obtain the same 1D plot from the simulated data, we used a position sensitive component with size 6 x 6 cm^2 (W x H), in compliance with the experimental configuration. The resulting data is a matrix of the neutron counts with a resolution of 0.1 cm. Subsequently the counts were summed along the columns (vertical axis; from -2.0 cm to +2.0 cm) and this gave a 1D array of the number of counts as a function of the horizontal position. In order to obtain the intensity in units of (neutron cm^{-2} s^{-1}) we had to divide the counts by the area across which the sum was made (i.e. 4 cm x 0.1 cm = 0.4 cm^2).