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The neutron guide upgrade of the TOSCA spectrometer

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ABSTRACT

The primary flightpath of the TOSCA indirect geometry neutron spectrometer has been upgraded with a high-*m* 14.636 m (including 0.418 m of air gaps) neutron guide composed of ten sections in order to boost the neutron flux at the sample position. The upgraded incident neutron beam has been characterised with the help of the time-of-flight neutron monitor; the beam profile and the gain in the neutron flux data are presented. At an average proton current-on-target of 160 μA and proton energy of 800 MeV (ISIS Target Station 1; at the time of the 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 a 3.0 × 3.0 cm^2 surface centred around the (0,0) position) is approximately 2.11×10^7 neutrons cm^{-2} s^{-1} while the gain in the neutron flux is as much as 46-fold for neutrons with a wavelength of 2.5 Å. The instrument's excellent spectral resolution and low spectral background have been preserved upon the upgrade. The much improved count rate allows faster measurements where useful data of hydrogen rich samples can be recorded within minutes, as well as experiments involving smaller samples that were not possible in the past.

1. Introduction

TOSCA is an indirect-geometry inelastic neutron spectrometer optimised for high resolution vibrational spectroscopy in the energy transfer region between −24 and 4000 cm^{-1} [1–3]. The instrument has been operational for almost two decades and during that time has set the standard for broadband chemical spectroscopy with neutrons [4]. In autumn 2013 as part of the international beamline review [5] it was concluded that for TOSCA to be able to participate in strategic research areas such as CO_2 capture and charge storage [6], an increase in the incident neutron flux *via* the provision of a neutron guide (as opposed to the simple collimation tubes present at the time) would be highly beneficial. Such a development would allow detailed studies of industrially relevant systems containing weak neutron scatters (SO_2, CO, NO) as well as faster parametric studies, particularly for hydrogen containing molecules such as hydrocarbons. Additionally, as neutron scattering is an inherently intensity limited technique, studies of smaller samples, which are too expensive to produce in larger quantities, would be possible. Since then, this major upgrade has been implemented which has involved extensive simulations together with the complete redesign of the TOSCA primary spectrometer to house a state-of-the-art, high-*m* neutron guide and associated chopper system to boost the incident flux on the sample.

Neutron guides are essential in order to boost the neutron flux at a long distance from the neutron source. As neutrons fly nearly parallel to the guide surface they are retained within the tube by a process of external reflection. Traditionally, neutron guides are square or rectangular cross-section tubes made from optically flat materials, usually glass, that has been metal coated with alternating layers of metal with different scattering length densities. More recently, and in particular for longer neutron guides, their shape can be rather complex (e.g. elliptical) in order to avoid the loss due to a large number of reflections. Over the years, progress in guide manufacture has led to supermirror coated guides, having high reflectivity and high *m*-values where $m = \gamma_c(\text{supermirror})/\gamma_c(\text{nickel})$ *i.e.* it is equal to the ratio of the critical angle of reflection, γ_c, of the supermirror and nickel coated optically flat glass [7]. The neutron guides with greater *m* factor lead

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to increased divergence of the neutron beam, for which the maximum value is given by the critical angle $\gamma_c[°] = 0.1 \times m \times \lambda$ [Å]. In our preliminary feasibility analysis of the TOSCA neutron guide we have excluded the use of elliptical or more complex geometries (that are more expensive to manufacture and may considerably increase the neutron divergence at the sample position) in order to concentrate our resources on a guide with an advanced supermirror coating. Thus we have used a tapered guide in order to focus the beam at the sample position while making sure to preserve the homogeneity of the beam.

Based on extensive neutron-transport simulations and baseline studies of the guide neutronic response [8–10], in this article we present the careful mechanical engineering design of the new TOSCA primary spectrometer and provide a review of the actual performance gains following this upgrade. A comparison between experimental observations and Monte Carlo simulations is provided, and the effect of the upgrade on the instrument spectral resolution and background have been assessed as well.

2. The primary spectrometer

In our design of the neutron guide, we have followed two principles: position the supermirrors to include as much of the neutron flightpath as possible, and to increase the area viewed of the water moderator by increasing the size of the shutter entrance (from its original value of 84 mm × 84 mm) while preserving the beam size at the sample position. A schematic drawing of the new 14.636 m long neutron guide (including 0.418 m of air gaps) which is dedicated to the TOSCA instrument is shown in Fig. 1. The first section of the guide, G1, is installed in the new 1.937 m long shutter that is positioned at a distance of 1.626 m from the moderator centre. The shutter contains an $m = 5$ straight square guide with an aperture of 100 mm × 100 mm. The remaining nine sections of the guide are tapered, starting from the 100 mm × 100 mm entrance of section G2, all the way towards the end of section G10 with 40 mm × 40 mm aperture (positioned at a distance of 16.262 m from the moderator centre, i.e. 0.748 m from the sample position). The angle of taper, ∼ 0.136494°, has been kept equal in each tapered section, while the *m*-factor was increased in steps from $m = 5$ for sections 2 to 6, $m = 6$ for sections 7 to 9, and $m = 7$ for section 10. This gradual increase ensured optimal gain and enabled that even those short wavelength (high energy) neutrons whose divergence was sufficiently small can be retained. Geometrical parameters of each section and the neutron guide as a whole can be found in Table S1 of the supplementary information. We have chosen mostly tapered over mostly straight guide as neutron simulations pointed towards increased flux gain in the case of the former [8–10].

As part of the upgrade, the current single disc chopper [3] has been replaced by a double disc chopper positioned at a distance of 9.455 m from the moderator centre, and between sections G5 and G6 of the guide. The air gap between the two sections required to fit the discs was kept to a minimum of 6.6 cm, thus reducing the neutron flux attenuation due to scattering by air. The new double disc chopper allows utilisation of all the neutron pulses arriving at TOSCA, even when Target Station 1 operates in 50 Hz mode (albeit without access to the elastic line; see reference 3 for further details about the extension of the spectral region of the instrument).

In order to achieve the highest neutron flux at the sample position, the flightpath through the neutron guide is in vacuum (p = 2.5×10^{-2} mbar). Since all the sections of the guide could not be joined together in a single housing, various housings are sealed with the help of 0.5 mm thick aluminium windows. Overall, there are a total of nine aluminium windows along the beamline flightpath (*i.e.* between the moderator and the sample position) as indicated by the orange vertical lines in Fig. 1.

Two neutron beam monitors are positioned along the flightpath; the first before the chopper, at a distance of 8.900 m from the moderator centre and the second after the chopper at a distance of 15.871m from the moderator centre. The latter monitor is used for the normalisation of the neutron flux. The monitors allow measurements of the time-of-flight spectra of neutrons; and were made from GS20 cubes (cerium-activated lithium aluminosilicate glass, 0.25 mm in size) that were distributed 7 mm apart and across a 7 × 6 array [11,12].

TOSCA has four ^{3}He detector tubes (two on each side of the beam) in back scattering that are used for diffraction measurements. As a result of the beam upgrade and in order to accommodate the last section of the guide they needed to be slightly moved away from the centre of the flightpath *i.e.* they are now positioned at an angle of 175°and 176°in the backward direction. Although the tubes are stationed in air, virtually all the flightpath between the sample position and the diffraction tubes is in vacuum, with the vanadium window acting as the boundary. The final section of the neutron guide, G10, is connected to the instrument by the tapered flight tube and the whole volume is kept at cryogenic vacuum (< 10^{-6} mbar).

The instrument was not operational between the end of May 2016 and mid-February 2017. By the end of November 2016, all sections of the guide were in place apart from the new TOSCA shutter with the initial section of the guide within it, G1, which remained the same as before the upgrade. Since the overwhelming majority of the guide was installed we tested the setup for enhanced neutron flux, in order to have better idea about the influence of the guide inside the shutter (installed subsequently) on the neutron flux, beam profile, spectral resolution and background (see SI). We will refer to this interim configuration as the C1 configuration, while the configuration before the upgrade (i.e. without the neutron guide) will be denoted as C0 [13]. The last section in the shutter was installed in January 2017 to give the final (so called C2) configuration. After the two weeks of commissioning measurements the instrument was returned to the user programme.

3. Experimental setup

The experimental setup used to measure the neutron flux at the sample position was described in Ref. [13]. The neutron sensitive component was a cuboid of cerium-doped glass scintillator, measuring 0.96 × 0.95 × 0.53 mm^3. The TOSCA closed cycle refrigerator (CCR) was 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. The position of this point-sampling detector was controlled *via* a computer script which moved it automatically after the accumulation of 10000 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. 169 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 every 5 mm, see Fig. S1 in supplementary information (SI). Subsequently the data were calibrated to give the neutron flux at the sample position in units of neutron cm^{-2} s^{-1} Å^{-1} and eventually integrated in the wavelength range of interest (see reference 13 for further details). At the time of this study, the first nine sections of the guide starting from the shutter towards the sample position were under vacuum, while section ten of the guide and the sample environment area were in air.

Computational details. The McStas software package [14] was used in order to perform Monte Carlo simulations of the TOSCA beamline. The geometrical parameters of the upgraded instrument primary beamline (see Table S1 in SI) were implemented in the virtual instrument, while the water moderator file [14] was provided by the ISIS Neutronics Group and was built using MCNP-X calculations of the actual TS1 target-reflector-moderator assembly. In the simulation the angle between the TOSCA beamline axis and the moderator face was kept at 90° *i.e.* the moderator face and the shutter face were perfectly aligned/parallel. In reality, the beamline axis is tilted by ∼ 13.2° from the line perpendicular to the moderator face [15] and this precise information has been taken