Tosca Secondary Upgrade

This project comes as natural consequence of the 2016 installation of a neutron guide on Tosca. This has been hugely successful and has enabled experiments that were previously borderline or impossible, such as molecules encapsulated in C_{60}, non-hydrogenous materials and much smaller samples. This project will replace the secondary flight path of the instrument with an analyser with a much larger collection area, while maintaining the current resolution. This will result in a gain in detected flux by at least a factor of 8 and 12-16 is conceivable. This would result in an overall gain, relative to the 2015 instrument, of ~100. This is transformative.

Summary of physical changes

The project will replace the existing 20-year secondary spectrometer on Tosca by one with a much larger collection area and with position sensitive detectors. The total collection area of Tosca at present is 1000 cm^2. By replacing the existing secondary spectrometer by one with a much larger collection area and optimised detectors, we can obtain a gain factor of at least 8 and potentially 12-16.

Science justification

The recent replacement of the previous straight tube by the installation of a high *m*-number converging guide on Tosca has dramatically increased the incident flux on the sample and, consequently, the signal-to-noise ratio (SNR). This was achieved while maintaining the existing, worlds-best, resolution of the instrument, which was a key requirement of the project. The increased flux has enabled experiments that were not previously feasible. An example is HD encapsulated in C_{60} (HD@C60). This sample only contains ~2 x 10^{20} H atoms, an order of magnitude lower than was feasible before the guide installation. But there is interest in even more challenging samples such as He@C60, this has an order of magnitude less cross section than HD@C60, so it is marginal whether it would be successful. Non-hydrogenous systems have always been challenging on Tosca; the guide has enabled measurements of ideal (*i.e*. bulk) samples of industrial and catalytic relevance such as $LiFePO_4$ and $K_2[PtBr_6]$, but to enable studies of real-world samples such as batteries (where the mobile species is Li, Na, or Mg ions) or direct observation of gasses relevant to climate change (CO_2, NO_x, SO_x) in the presence of hydrogenous materials, requires an order of magnitude gain in sensitivity. ISIS has a notable track record in high pressure science using diffraction instruments. Inelastic scattering has lagged in this area; the guide has made such experiments feasible, but they are very demanding because the sample sizes are very small, ~80 mg, and require a 24-hour measurement. To make such measurements even semi-routine necessitates an order of magnitude increase in SNR. As always, the trend is for increasingly demanding measurements. Whether this arises from low cross section, small sample size (or both) the only viable solution is increased sensitivity. The most effective way to increase the sensitivity of Tosca is to upgrade the secondary spectrometer.

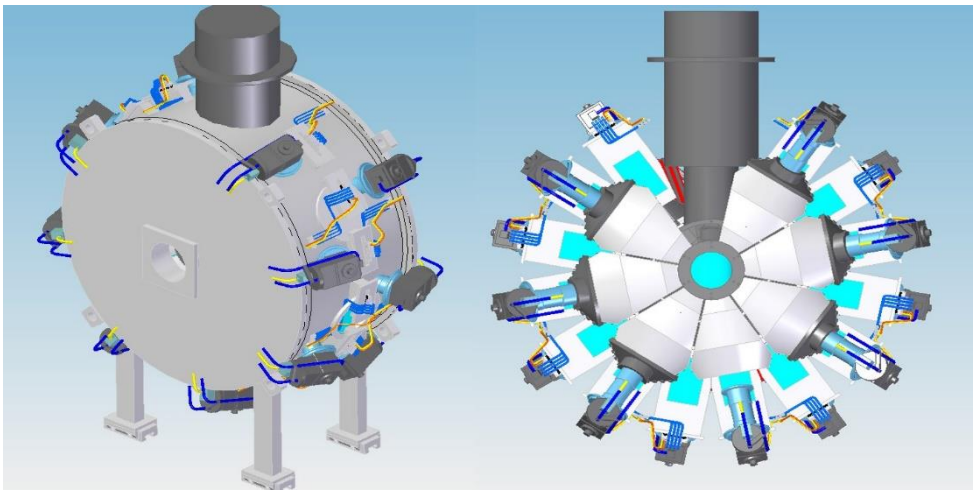
Business case

The Tosca spectrometer with the proposed upgrade fulfils STFC's strategic goals of world-class research, world-class innovation and world-class skills. Tosca's research outputs help solve real-world challenges by supporting academic and industrial projects (~25% of beam time has an industrial component). Tosca's research portfolio also fits well within STFC's industrial strategy, providing a truly unique method for the study of materials relevant to addressing the grand challenges, particularly for energy materials and Net Zero. The scope of the project covers the design, fabrication, installation, testing and safety requirements associated with the replacement of the existing 20-year secondary spectrometer by one with a much larger collection area and with

position sensitive detectors. The expected benefits are to improve the sensitivity, reliability, capability and capacity of Tosca, enabling the instrument to keep pace with developments at other facilities (Lagrange at ILL, Visionat SNS,

Vespa at ESS) and remain a world-class instrument. These benefits are to the user community (academic and industrial), instrument scientists and ISIS as a whole, with improved scientific output.

Summary of current status



Preliminary design of the new secondary spectrometer of Tosca.

A preliminary design has been made (see below), based on extensive McStas simulations of the instrument performance. There are some constraints to the project: the primary spectrometer will not be changed which means that the sample position cannot change. There is a physical constraint in that the footprint of the instrument must be largely unchanged. Our current estimates are that the project would be ready for detailed design by the end 2021. Assuming funding is available from early 2022, procurement would occur in 2022 and installation would be complete by the end of 2023.

The project will require significant effort from the Design and Detector Groups at a time when there is heavy demand for their services. The technical requirements associated with this project are well-understood (use of beryllium, position sensitive detectors) and are known technology, so that no developments are needed.

A gain factor of 8 or so is achievable by increasing the collection area. Simulations show that increasing the mosaicity of the graphite analyser crystals from 2° to 4° will double the detected flux *i.e.* a gain of 12-16 is conceivable. However, 4° graphite in sufficient quantity is currently unavailable.