SANDALS II

Next generation diffractometer for light-element-bearing disordered materials, delivering enhanced count rate, stability, real and reciprocal-space resolution, low backgrounds, and kinetic capabilities.

Summary of physical changes

1. Install new detectors in the banks left empty after the 2005 refurbishment
2. Upgrade existing detectors with up-to-date more efficient design
3. Replace argon boxes with NIMROD-style vacuum tank, encompassing sample + scattered flight paths
4. Install new detector bank around 90 degree scattering angles
5. Install new NIMROD-style sample access hatch to side of sample area

Excluded: Any front-end modifications to primary flight path (already included in interim upgrade)

Science justification

SANDALS has been a front-line ISIS instrument for 32 years and continues to deliver strong scientific output, impacting many fields and industries where molecular liquids and glasses play key roles.[1-3] The instrument is optimised for total neutron scattering measurements that are time-consuming to perform, especially when combined with the need to study many isotopically substituted samples to deliver the desired levels of structural insight. To date, the majority of studies on SANDALS have been limited to benchmark measurements in small regions of sample phase space, but there is growing **demand from multiple sectors for increasingly complex studies that currently cannot be met due to realities of the required measurement times.** A recent example of an investigation that has pushed the envelope of practicality was a study of **deep eutectic solvents for green materials synthesis**.[4,5] This project required measurements from 42 samples spread across two weeks of instrument time and multiple allocations – a clearly undesirable scenario.

Here we propose to upgrade SANDALS for increased sample count rates, by a factor ≥ 2.9, and that will give a total increase of factor ≥ 4.7 when combined with the results of the interim front-end upgrade that is currently underway. This will bring typical counting times per sample down from the current 5hrs to 1hr; achieved by increasing solid angle detector coverage (factor 2.3), detector efficiency (factor 1.25) and by improving signal-to-background (≥ 2 orders of magnitude). These gains will enable the study of compositionally complex materials and wider mapping of sample phase space, and deliver transformative changes to the instrument's programme in **amorphous pharmaceuticals, green solvents, battery electrolytes, thermal energy storage media, and homogeneous catalysts**.

This enhanced detector coverage will also improve the instrument's ability to perform **parametric, *in situ*, *operando* and time-resolved studies**, that are very important for **industrial and applied science programmes** where elevated temperatures, pressures, or sample compositional variation, are requested. This will facilitate the study of smaller or weaker scattering samples and open the door to **extreme conditions measurements** performed at pressures in the GPa range utilising the Paris-Edinburgh cell, or at temperatures in the 2000-3000K range using aerodynamic levitation. Furthermore, improved small sample capability will make possible studies that require expensive isotopic components that can only be purchased in small quantities, or of difficult to synthesize materials.

The incorporation of the proposed high-angle scattering bank (*circa* 90°) will notably enhance the instrument's ability to investigate partially ordered materials, and benefit studies such as *in-situ* crystallization of supercooled liquids, supersaturated solutions and glasses. Amongst anticipated beneficiaries, this capability is of importance for studies of **nanostructured catalysts, bioactive glass-ceramics, nuclear waste storage, automotive glasses and pharmaceuticals**. The 90° bank will also improve high-Q statistics for non-hydrogenous samples and will, for suitable systems, enhance real-space resolution and reduce measurement times yet further.

The project also aims to deliver improved access to the SANDALS sample point through provision of a side door on the instrument vacuum tank. This will simplify the installation of complex sample environment equipment, as well as multi-probe setups that combine neutron diffraction with ***complementary techniques such as Raman, UV-vis, or NMR spectrometry*** . In addition, beamline logistics will be improved by decreasing reliance on the crane, saving instrument scientist time (~50hrs/yr) and overall, contributing to the increased throughput, versatility and impact of the instrument going forward.

In practice, all of the upgrade solutions proposed above that are suited to individual science drivers will combine synergistically to enable a wide range of new research programmes.

Business case

The proposed upgrades will enhance the already strong reputations of ISIS, STFC and UKRI, whilst clearly fulfilling each of their vision and mission statements. This will be achieved both through enhanced scientific output toward clean economic growth and population health, but also through staff learning and development in instrument development and commissioning, that is important for the long term health of UK neutron scattering (ISIS-II), and research and innovation in general.

The proposed upgrades will enhance the position of SANDALS as the pre-eminent neutron diffractometer *worldwide* for study of disordered hydrogenous materials and allow it to better complement the capabilities of the other two Disordered Materials diffractometers at ISIS, NIMROD and GEM. SANDALS currently has an absolute count rate about half that of NIMROD (although it is better in the epithermal range that is critically important for total scattering), but this will be reversed post upgrades, making SANDALS-II the instrument of choice for time-resolved, parametric, large-sample set, low contrast or small samples on length scales up to 5nm. NIMROD will therefore benefit from greater capacity for its raison d'être in experiments requiring combined small- and wide-angle neutron scattering. Increased capacity on SANDALS-II will also benefit GEM by absorbing demand for non-hydrogenous amorphous materials studies, allowing GEM to capitalize on its higher *Q*-resolution for studies of disordered crystals.

Summary of current status

SANDALS-II is a replacement of the SANDALS instrument downstream of and including the sample area. This means a new vacuum tank with access port, low angle detectors, a 90° detector bank and a new counting house. Upgrades to the instrument upstream of the sample area are being installed during 2021 in an interim upgrade project. The vacuum tank and low angle detectors will largely be a complete copy of those used on NIMROD, and the 90° detector bank will be based on technology established on other ISIS instruments.

The biggest design challenge will be fitting the NIMROD-style vacuum vessel and detectors inside the current SANDALS blockhouse, requiring some alterations to the blockhouse. The 90° detector bank needs to be considered, as the plan is to position it by the sample area on the side nearest ALFRED. If it does not fit in the available space the blockhouse would need to be extended into the area currently used by the ALFRED intermediate shutter. An alternative would be to move the 90° to the other side and remove the sample access port from the specification.

The next biggest design consideration will be maintenance access for the detectors and vacuum vessel windows. This may involve adding access to the blockhouse on both sides of the instrument and ensuring the detectors and vacuum vessel can be craned out of the blockhouse to maintain the vacuum vessel windows.

Aside from these challenges the status of SANDALS-II is very promising, as it uses established technology that has previously been manufactured and installed successfully. This means the technological risks are very low.

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[1] A. K. Soper, Chem. Phys. **258** (2-3), 121 (2000). [2] C. Hardacre et al., J. Chem. Phys. **118** (1), 273 (2002). [3] R. Hayes et al., Phys. Chem. Chem. Phys. **13** (8), 3237 (2011). [4] O. S. Hammond, D. T. Bowron, and K. J. Edler, Angew. Chem. Int. Ed. **56** (33), 9782 (2017). [5] N. López-Salas et al., ACS Sustain. Chem. Eng. **7** (21), 17565 (2019).