LMX

A new single crystal diffractometer optimised for studies of large molecule systems, with applications across a range of research areas in the fields of macromolecular chemistry and structural biology.

Summary of physical changes

The project is to construct and commission a new single crystal diffractometer, LMX, on the ISIS Second Target Station. To meet the demands of the science and business cases outlined below, the design of LMX includes a long incident beam path and novel neutron optics, allowing the diffractometer to be highly optimised to deliver a high flux of cold neutrons and to resolve low d-spacing Bragg reflections from very large unit cell crystals. The instrument will be a world-leading single crystal diffractometer, ideally suited to the second target station at ISIS.

Science justification

Structure determination by single crystal neutron diffraction has proved to be a highly successful technique for many decades, originally at reactor-based (monochromatic) facilities and then at spallation (pulsed) sources. Whilst the SXD instrument at ISIS has made significant contributions in the area of 'small molecule' chemical crystallography (with unit cell volumes typically up to around 10,000$Å^3$), the past 20 years or so has seen increased demand for the study of larger molecular systems. LMX will be designed to accommodate unit cell volumes up to ~2,000,000 $Å^3$, a 200-fold increase on SXD. This includes many topical research areas, such as supramolecular chemistry, hybrid organic-inorganic complexes that exhibit mixed properties, molecular magnets, zeolites and other framework materials (e.g. Metal Organic Frameworks, MOFS), energy harvesting materials, organometallic chemistry, catalysis and biomolecular science (recent examples being, studies of the active sites of HIV and SARS-CoV-2 proteases for developing new drug inhibitors). These, and other, potential science areas to be studied on a future LMX were highlighted during a European Neutron Diffraction single-crystal workshop (ENDic1), organised by the ISIS Crystallography Group at Cosener's House, Abingdon in April 2017 (http://purl.org/net/epubs/work/43907554).

The vast majority of structural studies of large molecule systems are performed using X-rays at synchrotron sources. For example, Diamond has a suite of macromolecular beamlines dedicated to solving the crystal structures of large molecule systems using single crystal diffraction. However, the X-ray technique does not provide information on the location of light atoms in the presence of heavy ones (in particular hydrogens which are often the key to understand interactions in biological processes and drug binding sites, but also oxygen atoms or small cations hosted in MOFS), nor can distinguish between isotopes of the same element. Given this natural complementarity between neutron and X-ray diffraction methods, we will develop a close collaboration with Diamond. Furthermore, we are working to create collaborative links with the Rosalind Franklin Institute, currently under construction on the Harwell Campus.

Business case

At present, ISIS has only one dedicated single crystal diffractometer, SXD, which has a scientific programme focussing predominantly on chemical crystallography, with some additional interest from the physics and materials science communities (spin-ices, incommensurate structures and shape memory alloys) and diffuse scattering studies of organic and inorganic materials.

A programme to upgrade the detector complement of SXD is underway, which will increase its countrate by a factor of approximately three. However, even with the upgrade of the detector system, SXD will not be able to tackle molecular systems with unit cells larger than a few tens of thousands of $Å^3$, and will not be able to address the scientific problems outlined in the previous section. Thus, the construction of an LMX instrument will expand the capabilities offered by the ISIS Crystallography Group, meeting the needs of a new family of external research groups whose requirements cannot currently be met at the facility.

Beyond ISIS, within the European neutron landscape many current single crystal diffractometers are located at reactor-based facilities, such as the ILL. As these sources are scheduled to close over the coming decade or so, there will be a shortage of provision in this area (even with the start of operations at the ESS, its two planned single crystal machines cannot fulfil the needs of the user community). Thus, we foresee that significant demand for LMX will be drawn not only from the UK community that presently uses the ILL for their experiments, but also from research groups outside the UK.

Plans for a dedicated single crystal macromolecular beamline on the Second Target Station at ISIS have been discussed for many years, with an outline design and a proposal originally submitted as part of the Phase-II instrument development suite in 2005. However, the project was not approved at that stage. Whilst the scientific case was adjudged strong, there were technical concerns - especially around the provision of suitable two-dimensional detector technology. In the past few years, significant advances have been made in this area by the ISIS Detector Group. A prototype two-dimensional position sensitive detector module based on Wavelength Shifting Fibre (WSF) technology has recently been installed on SXD and has already shown excellent performance in terms of efficiency and spatial resolution. As a result, the ISIS Crystallography Group has revisited the scientific and business cases for an LMX diffractometer and is in the process of optimising the technical design, to take advantage of the progress made in detector technology and other areas, such as neutron guides.

Summary from engineering side on status of design, costing and schedule

LMX is a completely new instrument to be constructed on the vacant TS2 Port-W3. The design of the main instrument up to the sample area is yet to complete as it is dependent upon simulation work, which is anticipated to occur during2021.

The project is a 3.5 year project, comprised of 3 main over-lapping project phases, each of approximately 1.5 years duration: design; manufacture; installation. IDD Instrument Section has confidence in designing and constructing LMX, due to the similarities with WISH (I and II), incorporating the lessons learnt on WISH-I over years of operation, guided by the experienced instrument scientists, combined with a construction on a ‘green-field’ site.