HRPD-X

A major upgrade to the current HRPD instrument at ISIS, to expand its user base into new research areas and maintain its position as a world-leading facility for high resolution powder diffraction using neutrons.

Summary of physical changes

The High Resolution Powder Diffraction (HRPD) instrument is a long-established ISIS instrument and is a flagship for both the facility, STFC and the UK powder diffraction community, whilst also setting a benchmark for high-resolution instruments elsewhere in the world. It has undergone a number of upgrades during its life-time, the most significant being a replacement of the neutron guide in 2007. However, the detector suite and vacuum vessel still reflect the original 'day-one' concept, using 1990s technology. Consequently, these key components are showing clear signs of age and are in need of upgrading/replacement. An HRPD Interim refurbishment project was carried out in 2019 as an urgent measure, primarily to replace at-risk electronics, in order to sustain the instrument and its user programme until a full upgrade could be undertaken. However, this refurbishment did not provide any enhancement of the instrument's scientific capabilities.

The proposed upgrade is a rebuild of the instrument beyond the end of the neutron guide, to finally exploit the gains in neutron flux provided by the 2007 guide replacement. It is planned to replace the current detectors with state-of-the art wavelength-shifting fibre-based technology and associated electronics, providing improvements in detector reliability and stability. However, the major advance in instrument performance will come from a significant increase in detector solid angle (by a factor of four overall and with a 90-fold increase at $2\theta < 80°$) whilst maintaining the current high $\Delta d/d$ resolution. An equally important addition will be improved collimation of both incident and scattered beams, reducing background scattering especially when using complex sample environment devices. For the scattered beam, it is proposed to install a static radial collimator, as these devices have proved highly effective at significantly reducing parasitic scattering from sample environment surrounding the sample on GEM, WISH and Polaris. The plan is to create a vacuum tank for the scattered beam by utilising thin windows and a small vacuum volume to minimise attenuation and retain quick pump-down times. The remainder of the flight path to the detectors will be through argon-filled tanks. To accommodate the new detectors and collimation, it will be necessary to replace the existing evacuated sample tank with a new one lined with B_4C to reduce neutron backgrounds and fitted with a vacuum system for rapid pump-down. This will also be non-magnetic to enable use of fields up to 10 T (not possible at present). Finally, to accommodate the upgraded instrument and improve the working environment, it will be necessary to completely rebuild building R69, and a detailed layout and costing has been developed in collaboration with a team of external architects.

Science justification

The powder diffraction community is amongst the largest and most productive at ISIS, being drawn from diverse fields covering chemistry, physics, materials, earth and planetary sciences, engineering and cultural heritage research. As mentioned above, the main objective of the HRPD upgrade project is to provide a whole new facility, which builds on the scientific distinction achieved over the past 35 years of HRPD's operation, whilst also seeking to expand that standard of excellence across new areas of materials science,

physics and chemistry for decades to come. The excellent direct-space resolution provided by HRPD has proved to be a powerful tool to understand subtle structural phenomena, often related to important scientific or technological properties. HRPD has been a flagship instrument for ISIS and the UK user community, with highlights including very highly cited papers on C_{60}, $YBa_2Cu_3O_{7-x}$, multiferroic $BiFeO_3$, pnictide superconductors, and negative thermal expansion materials.

The proposed upgrade to the detector complement on HRPD, including tailored in-beam collimation and a non-magnetic tank, will expand its scientific domain into many areas, including high resolution studies of more

complex organics and inorganics; catalytic materials (molecular sieves, zeolites and microporous solids); organic-inorganic composites (clathrates, inclusion and intercalation compounds); metallic, organic and ionic magnetic materials with incommensurate nuclear and magnetic structures and/or large unit cells (multiferroic compounds, complex organic systems, highly hydrated inorganic salts, magnetic materials); strain and phase separation studies (engineering applications, in-situ determination of ferroic hysteresis, structure-property relationships); high-pressure neutron studies at higher resolution than currently available (multiferroic compounds, planetary materials, complex organic molecular systems, magnetic systems); measurements using applied fields in complex sample environment (engineering stress measurements, parametric studies of multiferroic compounds, ferroelectric compounds, magnetic materials, and ferroelastic phases); rapid parametric studies at high resolution (as a function of temperature, pressure, chemistry etc.); complex in-situ studies (under flowing reactant gases including controlled fugacities and humidity, battery materials under charge and discharge conditions, ion exchange, hydrothermal syntheses) and studies of small samples (e.g. isotopically enriched compounds, materials prepared by pressure/temperature quenching from multi-anvil presses).

Business case

Whilst HRPD has undergone a series of sequential upgrades in the roughly 30 years since its 'day-one' configuration, many of its key components, including the sample tank and detector system, are showing clear signs of age; moreover, these are ill-suited to the expanding needs of the user community. The upgrade to the HRPD instrument will greatly enhance STFC's neutron facility, leading to improved instrument performance, in terms of reliability and enhanced scientific capability. The upgrade is essential to maintain HRPD's place at the forefront of the world-wide diffraction community in the face of increasing competition from new high resolution powder diffractometers at the SNS, J-PARC and ESS.

Summary of current status

HRPD-X has been in Concept and Definition stages for some years now and as a result the design is quite advanced. The building design work has almost cleared the design stage and we are awaiting professional QS estimates for timescales, costs and a spend profile that we will communicate to IMC in March via the project's Life Cycle Document. In April we hope to proceed to the new HRPD-X building's detail design.
The instrument design is on-going within IDD and all areas are progressing well. Though some tasks are challenging, they are still interesting and there are no concerns over any aspects of HRPD-X's design.