ANNEX I

Instruments and instrumentation development

Below is a list of potential areas for collaborative development of instruments and instrumentation.

Target Station 1

A) INES operation

INES is the experimental station operated under the scientific leadership of CNR. CNR will allocate 100 k€ per annum to STFC for the salary of the INES instrument scientist and to maintain and operate the INES beamline at ISIS. ISIS will hold this money on behalf of CNR acting as paymaster in respect of the costs to be met on CNR's behalf.

A) TOSCA upgrade.

The TOSCA spectrometer at ISIS was funded by the CNR to replace its predecessor TFXA. TOSCA remains to this day the highest-resolution inelastic neutron spectrometer in the world over an unrivalled energy-transfer range (25-4000 cm^{-1}). As such, it represents a superb example of the unique capabilities afforded by short-pulse spallation techniques, e.g., tight (chemical) resolution over a broad spectral range.

An upgrade of the TOSCA spectrometer on ISIS-TS1 will be transformational for the chemical sciences. Detailed neutronic simulations as part of on-going collaborative efforts between ISIS and CNR team have established that use of present neutron-guide technology in the primary instrument will deliver a 1-2 order-of-magnitude increase in detected flux on this instrument. This new capability will be transformational, enabling the chemistry community to tackle materials-chemistry challenges of direct relevance to societal needs and long-term economic sustainability. These include: gas sequestration by nanoporous media e.g., uptake of flue and greenhouse gases like carbon and sulphur dioxide by metallo-organic frameworks; the rational design of graphene-based nanostructures and nanocomposites for next-generation carbon-based functional materials and sensors; chemical catalysis of industrial relevance, including the synthesis of biomolecules like vitamin A using Lindlar-type catalysts or iron-based Fischer-Tropsch catalysts for the efficient liquefaction of coal to make synthetic fuels; new charge-storage and fuel-cell materials relying on the transport properties of light atoms such as hydrogen or lithium at intermediate temperatures; and a plethora of advanced materials such as negative-thermal-expansion materials or thermoelectrics.

B) Improved Engineering Diffraction Instrument.

ENGIN-X is a world class dedicated engineering instrument. There are primarily two types of experiments carried out on ENGIN-X - residual stress measurement and in-situ experiments to observe micromechanical properties of material. The success of ENGIN-X is based on : (*i*) continually development to make the use of instrument more user friendly (*ii*) offering a wide range of sample environment equipment (*iii*) a dedicated and expanding user community especially in the area of industrially applied research. At present the oversubscription is a factor of approximately five, with a significant demand from industry enabled through a new access scheme pioneered at ISIS. This level of oversubscription is now detrimental to the academic and industrial user community. To satisfy both the capacity and capability demands requires a new instrument to complement ENGIN-X.

A new facility (preliminary name ENGIN-XXX) with the capability for residual stress measurement will serve the growing user community. The specification for the new instrument has similar (or better) resolution to ENGIN-X combined with increased flux. The resolution of the current ENGIN-X meets the present demand for residual stress measurements. However for approximately 10% of the in-situ loading experiments there would be significant benefit from improved resolution. The new instrument would provide enhanced capabilities to measure thicker samples (an important capability for real world engineering), improved 2D/3D mapping, and enhanced time resolution for in-situ experiments.

Together with ENGIN-X and IMAT (operational 2015) the new instrument would provide ISIS with a unique suite of capability and capacity to address the increasing challenge of materials engineering.

C) New interdisciplinary instrument developments on INES

Neutrons have the capability of penetrating several centimetres of material, and therefore are particularly suitable for the study of thick artefacts (e.g. metal objects, marbles, pottery, etc.), or thick processed food (e.g. contaminants for food safety assessment) that cannot be studied with other techniques (e.g. X-rays). Areas of application of non-destructive integrated neutron and optical methods include radiation issues on artefacts, transport in security, dating of biological specimens for biodiversity conservation and bio-geography, fraud stalking in food science. These applications are underpinned by the development of the associated hardware and software, data analysis protocols, and new optical-detection schemes. Areas of science and technologies envisaged include:

a) The integrated system for imaging of materials/artefacts making use of particle (neutron) and light probes. We will take advantage of the unique penetration properties of neutrons combined with the different penetration of electromagnetic radiation, to build a tomographic image of the samples under study. The neutron component will be at first a specific development of the INES beamline and subsequently for IMAT beamline. The light component and related detection systems will be based on optical-radiocarbon-dating methods, i.e. optical $^{14}C^{16}O_2$ detection for on-site dating. It is intended to develop a prototype of a new apparatus for optical detection of $^{14}C^{16}O_2$, based on saturated-absorption cavity ring-down (SCAR) spectroscopy, much more compact, easier and cheaper than the one already developed for laboratory use [Galli et al., Phys. Rev. Lett. **107**, 270802] at the Institute CNR-INO in Florence. The implementation of a transportable version will be developed to operate on site at ISIS for the analysis of archaeological objects, for the dating of cultural heritage samples. In particular, the 4.5-μm laser source will be simplified, moving from the intra-cavity difference-frequency generation referenced to an optical frequency comb in the near IR to a system based on 2 quantum cascade lasers directly emitting in the mid IR. One of them will be frequency locked and spectrally narrowed to a molecular line, while the other one will be scanned across the target $^{14}C^{16}O_2$ line. The cooling system relying on dry ice at 195 K will be replaced by a cryogen-free Stirling refrigerator, capable of cooling the spectroscopic cell down to 170 K, thus further suppressing other molecular lines interfering with the target one. The volume of the sample gas cell will be reduced from about 8 L down to 0.7 L and, correspondingly, the carbon mass required for the measurement from about 70 mg down to 6 mg. The overall size of the opto-mechanical setup (including cryo-cooling) will be about 120x100x70 cm^3 volume and about 100 kg weight. The laser current/temperature drivers, the locking electronics, the data acquisition/processing electronics and the vacuum pump will be hosted in a 19" rack mount with about 180 cm height and about 100 kg weight. The sample preparation, cleaning and combustion will be the same as for accelerator mass spectrometry (AMS), performed by a commercial elemental analyser (EA), but with no need for graphitization of the obtained CO_2 sample. The overall cost of the new setup for $^{14}C^{16}O_2$ concentration measurements will be reduced from about 300 kEuro to less than 100 kEuro (not including the EA). We expect to improve the present sensitivity of 2 pMC (percent modern carbon), approaching the 0.3 pMC achieved by state-of-the-art AMS. This equipment is intended to operate in-situ at the ISIS beamlines for analysis and dating of archaeological samples. It will be installed on INES then on IMAT.

b) The knowledge of the elemental composition of samples is a valuable information in archaeology, providing insights into the production process and the provenance of archaeological artefacts. A research program in this area will be built on the instrumentation and methods developed within the Ancient Charm project [E. Perelli Cippo et al, Nucl. Instrum. and Methods in Phys. Res. A623 (2010) 693–698]. The work program will combine non-destructive techniques based on neutron sources, namely neutron resonance transmission and prompt gamma-ray activation analysis, to enhance the identification of specific elements and isotopes in artefacts. Both resonance energy patterns and neutron capture gamma-ray energies will be used to enhance isotopic identification and pinpoint the position of the elements in archaeological artefacts and in living and processed biological material. Neutron techniques also allow identification/detection of rare elements (lanthanides or rare earths) that can be at the basis of a next generation of traceability strategies for major agricultural commodities, food and any other biological material of plant origin, including wood. Rare earth spectra, when properly investigated may in fact reveal specific features in the biological matrix, allowing exact identification of geographical provenances. This is of special importance for niche productions with high added value [Bentil et al., J. Braz. Chem. Soc. **22**, 2011, Cobb, Analytical Chemistry **39**, 1967, Cullers et al., Chemical Geology **70**, 1988]. To take advantage of the full incident beam area, INES will be upgraded with a 2D position-sensitive neutron detector previously developed for the Ancient Charm European project. Further enhancements to INES include the installation of a high-resolution germanium gamma-ray detector to monitor the energy and time of gamma-rays following neutron capture. The detector will also be available for gamma-ray background studies in different beamlines and beamline ports at ISIS.

D) Optical and neutron integrated methods for excited states neutron spectroscopy

Neutron probing of the excited states of molecular systems can provide a direct access to the quantum states of reactive and highly mobile groups such as O-H in water, that initiate the proton transfer reactions, as well as the modification of the interatomic van der Waals potentials in the light-excited states in noble gases. Feasibility tests will be made in order to develop the methodology and techniques for simultaneous laser excitation and pump-probe measurements, and neutron scattering measurements of atomic and molecular systems in the excited states, giving access to a description of the quantum states involved. This activity requires the development of dedicated techniques and set –up such as:

- transportable laser instrumentation for the operation at the ISIS neutron beam lines for simultaneous neutron-laser measurements
- dedicated neutron sample containers with optical windows
- integrated pulsed neutron/pulsed laser acquisition systems

Target Station 2

E) Commissioning and exploitation of CHIPIR.

CHIPIR is the first beamline at ISIS designed for chip irradiation with fast neutrons. It will come into operation in 2014. The commissioning of the new beamline will be performed in two stages before and after the beryllium reflector replacement. New detectors for fast neutron spectrometry will be deployed. The instrumentation in support of chip monitoring during irradiation will be commissioned and made more user friendly in the first few years of operation of the beamline.

F) Commissioning and exploitation of IMAT.

IMAT is the first beamline at ISIS optimised for energy selective imaging. It will come into operation in 2015. The IMAT imaging system features energy selective imaging. The latter requires further development which can be addressed during IMAT commissioning and in the first years of operation of the beamline. Improved resolution detectors will be used as they become available. The diffraction detector banks will be completed.