Diamond Beamline Proposal 057

IXS: A Two-Branch Beamline for Inelastic X-ray Scattering

A proposal prepared for the SAC March 2011
1. Executive Summary

We propose to construct a two-branch beamline that will be Diamond’s first and only inelastic x-ray scattering (IXS) facility. The broad range of science areas that are accessible with the beamline cover some of the most interesting and topical, as indicated below. All other major synchrotron radiation facilities have—or are building or planning—instruments in this area, and IXS beamlines are the most highly oversubscribed by users.

The current proposal describes a scientific technique which is not available in the UK, although it has been developed at most synchrotron facilities and has become an important probe to determine the basic structure of low energy excitations in materials. It is supported by a wide range of research groups, some of which have extensive experience of using inelastic neutron scattering (INS). This technique is very well established in the UK and experiments have been performed on many strongly interacting electronic systems. Important complementary information can be obtained from IXS experiments, a technique in which several UK groups have gained valuable experience at the ESRF. Other groups have research interests based on materials that are prime candidates for novel investigations with IXS, such as the dynamics of interfaces and surfaces and the dynamics of carbon nanotubes and graphene. As with any new scientific facility, it is expected that its availability will stimulate many other research groups to work in this growing and important field, and that Diamond will become one of the main centres for IXS in Europe.

We are proposing two independent instruments. The first (SIX) is a soft x-ray branch with a long exit arm spectrometer located in a new external building. The second branch uses hard x-rays and will focus initially on a medium resolution spectrometer (MIX), mainly for resonant scattering but also suited to carry out non-resonant inelastic x-ray scattering (NrIXS or Raman scattering). It will furthermore accommodate the development of novel optics for a high resolution spectroscopy (HIX) using the same hard x-ray branch. The expected parameters for these instruments are listed in Table II.

To summarize, we propose:

- The only inelastic x-ray scattering facility in the UK.
- Two independent end-stations, to be operated simultaneously.
- A world-leading soft x-ray spectrometer to support a vibrant UK community in magnetic and electronic properties of novel solids.
- A hard x-ray branch to provide a world-class resonant inelastic scattering facility and future very high resolution non-resonant inelastic scattering, to provide new opportunities and research directions in the UK.
- The resolution of both end-stations will exceed those of currently operating spectrometers.

Acknowledgements

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academic research groups and industry.

2. The Scientific Case

2.1 Introduction

X-ray inelastic scattering is a new tool for studying problems in physics, chemistry, materials, geology and biology. The reason it was not developed earlier is that typically x-rays have an energy of several keV whereas many excitations of importance for understanding problems in condensed matter typically have energies between 1 meV and 10 eV. The implication of this large difference is that the energy of the incident and scattered x-ray beams must be exceptionally well defined, to say 1 part in $10^5$ or better, to enable the measurement of the small changes in the energy of the scattered x-rays. It is only since the development of third-generation synchrotron facilities producing intense and highly collimated x-ray beams that such experiments have become feasible for a wide range of different materials. Furthermore the x-ray optics for obtaining sufficiently monochromatic x-ray beams needed to be developed and this development continues to progress.

The simplest process by which x-rays are scattered is from the charge density of the electronic distribution of a material, which is called Thomson scattering. Almost all the crystallographic structures that have been solved using x-rays make use of this cross-section. The simplest inelastic experiments exploit the same scattering process. For example, instruments built at the ESRF have enabled the phonon dispersion curves of many materials to be obtained using IXS. This type of experiment is similar to that used for many years by inelastic neutron scattering. The energy resolution and count rates, currently obtained at the ESRF, are very similar to those obtained using neutron scattering techniques. A particular advantage of using x-rays is that much smaller samples are required, opening up many new materials for investigation. The different kinematics of the scattering also enable experiments to be performed at smaller wave vectors than is possible with neutron scattering and consequently a large number of important experiments have been performed on glasses. The small size of the x-ray beam opens up the new field of inelastic scattering from interfaces and surfaces. For all of these experiments the results are not critically dependent on the incident x-ray energy and the cross section is well known and understood. This technique is known as Non-resonant Inelastic X-ray Scattering (NrIXS).

Many properties of materials depend on the electronic excitations and an understanding of their nature is essential if many of their properties are to be understood. Examples are the $d$-$d$ transitions in materials with $3d$ electrons, charge-transfer excitations and orbital excitations; all of which cannot be observed with conventional infra-red and optical spectroscopy. Because the electronic excitations often involve the excitation of a single electron, the intensity of the x-rays due to Thomson scattering is very small, compared with the scattering by the phonons or by the multi-phonon spectra. This is particularly the case for materials containing heavy ions such as lead or the actinides. The problem is particularly severe for magnetic materials because the excitations are dependent on the electron spin and the interaction with the x-rays is orders of magnitude smaller. Nevertheless some experiments have studied the electronic structure using Thomson scattering because it is well understood and quantitative calculations can be made.

The drawback of the weak scattering can be surmounted, however, by using the resonant scattering from the excitations. This scattering uses an incident x-ray energy that is resonant with a particular energy transition in the system. The advantage of this technique is that the choice of the resonant energy implicitly means choosing a specific atomic core level in the sample. The excitations measured are then associated with only that particular atom and the selection rules depend on the electronic transition that was chosen for the resonance. This type of experiment is known as...
Resonant Inelastic X-ray Scattering (RIXS) and has been very successfully employed, notably at the Swiss Light Source (SLS) where measurements have been made of spin waves and other electronic excitations. The technique requires the ability to accurately control and adjust the incident energy such that the incident x-ray beam is at resonance with the electronic transition from the core level. At the SLS the instrument uses soft x-rays with energies between 0.4 and 1.8 keV. The incident energy can thus be tuned to the $L_{2,3}$ edges in $3d$ materials or the $M_{4,5}$ edges in $4f$ materials. Similarly, using a beamline with an incident energy between 5 and 20 keV enables experiments at the $K$ edges of $3d$ materials and the $L_{2,3}$ edges of $4f$ materials. Experiments at the SLS (ADRESS), APS (30ID, 9ID) and Spring8 (BL11XU, BL12XU) have shown that this is a powerful technique that gives a greatly enhanced intensity so that measurements can be made of the momentum, energy and intensity of the scattering from the electronic states for excitations between 50 and 600 meV for soft RIXS and from 0.1 to 20 eV for hard RIXS. At present the theory of resonant scattering is still in its infancy and so it is uncertain whether or not certain excitations can be observed. We anticipate, however, that over the next few years much progress will be made, partly through theoretical efforts—there is a large interest from theorists—and partly because more samples will be measured.

This proposal puts forward a plan for the instrumentation and developments that are necessary to provide state-of-the-art instruments for IXS at Diamond. The incident x-ray energy needs to be varied between 0.4 and 20 keV. Since x-rays strongly absorb for energies below ~2 keV two instruments are required. The first one is a station for soft x-rays (SIX) and will be in high-vacuum without any windows in the beamline while the other one is for hard x-rays (MIX) that will be in air behind a Be window in the beam line which will allow more sophisticated sample environments.

Resonant scattering can be measured using both the soft (SIX) or the hard (MIX) x-ray instruments. The choice between the two branch lines depends on the resonant process chosen so as to optimize the intensity and/or the resolution. The soft x-ray instrument has a monochromator that can adjust the incident x-ray energy to resonance energies below 2 keV and an energy analyzer with a resolution of $\sim$10 meV covering the $3d$ transition metal $L_{2,3}$, rare earth $M_{4,5}$, actinide $N_{4,5}$ resonances and the O, Mg, Al and Si $K$ edges. It is expected that the spectrometer will be able to measure excitations with energies up to 500 meV or more with a total energy resolution between 20 and 50 meV, operating mainly in a resonant mode.

The high energy medium resolution instrument (MIX) provides an incident energy between 5 and 12 keV and covers the $K$ edge of $3d$ elements and the $L_{2,3}$ edge of $4d$ and $4f$ elements. The spectrometer system will be very similar to that of the APS MERIX beamline (Figs. 6 and 7) providing (with interchangeable analyzers) an energy resolution of $\sim$50 meV mainly for applications of resonant scattering, but also allowing NrIXS measurements with an energy resolution in the range 50-150 meV. Furthermore, the hard x-ray branch will serve as a test-bed for the development of a high resolution spectrometer (HIX) with a resolution of $\sim$1 meV that will mostly be used to measure phonons and other low-energy excitations but normally not at resonance. This instrument accepts various sample environments such as low and high temperature stages, pressure cells and magnetic fields. Further refinement of the technique involves exploiting the polarization of both incident and scattered x-rays which would provide additional information by applying the selection rules for the transition probabilities.

NrIXS can be used to study valence- and weakly-bound-electronic excitations in materials. These investigations focus on obtaining a deeper understanding of the band structure and electron correlation effects. For example, although soft-x-ray absorption spectroscopy (XAS) is a powerful technique that enables the ground-state structural properties to be determined accurately, it is not well suited to determine the energies of the low lying excited electronic states because the energy width is limited by the core-hole lifetime and furthermore the energy of the final state is modified.
by the core-hole potential. In contrast, with IXS the low-energy excitations can be measured without these complications. NrlXS from the relatively low-energy electrons is also called x-ray Raman spectroscopy and is a rapidly developing and powerful technique for chemistry, physics and materials sciences, which is used to study low-\(Z\) materials, \(M\) edges of transition metals, \(N\) edges of rare earths and \(O\) edges of actinides. X-ray Raman scattering is also useful in providing structural information for disordered systems that can be an important complement to the information that is obtained from diffraction experiments.

2.2 The prime advantages of inelastic x-ray scattering

2.2.1 All inelastic x-ray scattering techniques

- The energy of the excitations that can be studied ranges from 1 meV up to several keV (Fig. 1).

- Momentum conservation allows the measurement of the dispersion relations for phonons and electronic excitations.

- The energy of the x-rays is much larger than the excitations being measured so that the instrumental resolution does not change as a function of the energy transfer, unlike in the case of neutron scattering.

- In the scattering process, both the energy and momentum transfer can be varied independently and the results are complementary to those obtained by inelastic neutron scattering, Brillouin scattering and infra-red/optical/x-ray absorption. However, in contrast to these techniques, with a high resolution spectrometer (HIX), momentum resolved information can be assessed in a broad momentum transfer range.

- Because the photon has zero mass, the kinematics of the scattering is different from that of neutron scattering. This enables measurements to be made at smaller wave-vectors than with neutrons.

- The second-order scattering process provides more information than x-ray absorption spectroscopy (XAS) or x-ray photoemission spectroscopy (XPS), for example, \(d-d\) transitions are allowed in IXS but electric-dipole forbidden in optical transitions.

- IXS can be used to measure the bulk properties of a sample as well as the buried interfaces (up to several microns deep with hard x-rays).
• Using the photon polarization the symmetry of the ground state can be determined by analysing the excited states.

• Only small sample volumes are needed so that measurements can be performed on materials that cannot be obtained in large quantities or in constrained sample environments, such as under high pressures in a diamond anvil cell (DAC) and encapsulated samples containing, for example, gases or actinide elements.

• The spot size of the x-ray beam can be as small as a few microns which will allow the determination of the excitations associated with surfaces, interfaces, nano-objects, small crystals and ferromagnetic and electric domains.

• The incident and scattered photon beams carry no charge or spin so that experiments can be readily performed in the presence of electric and/or magnetic fields.

• The variation of the cross section with atomic number is very different from that of neutrons. Materials that have prohibitively large absorption coefficients or incoherent scattering lengths for neutrons can be studied with IXS. This is the case for samples containing elements such as B, Gd or Cd.

2.2.2 Non-resonant inelastic x-ray scattering (NrIXS)

• The measured IXS cross-section is proportional to the dynamic structure factor for phonons or electrons, which enables a direct comparison of the experimental results with theoretical calculations. Furthermore the scattering depends on the energy transfer and wave-vector transfer but not on the particular energies and wave-vectors of the incident and scattered x-rays.

• Since the energy of either the incident or scattered x-rays need not be varied during these experiments they are technically more straight forward, which can be used in advantage e.g. to increase the energy resolution.

2.2.3 Resonant inelastic x-ray scattering (RIXS)

• Because the incident energy is in resonance with the electronic core to valence transition the intensity of the scattering is strongly increased, often by many orders of magnitude.

• The dispersion curves for magnetic excitations can be measured.

• By tuning into the appropriate absorption edge the enhanced cross-section can be made element-, site-, shell- and symmetry- specific.

• Sum rules for the integrated intensity over a specified decay channel can be used to determine the magnetic properties of the local ground state of the absorbing atom.

• Measurements can be made with the energy resolution less than that of the core-hole lifetime of the intermediate state.

2.3 Science enabled by inelastic x-ray scattering

The science that can and will be carried out using IXS is vast and diverse and can be classified in many different ways. We have chosen classify using traditional disciplines such as Physics, and
Chemistry but one of the important features of x-ray scattering is that many of the possible experiments are interdisciplinary and that the users will come from all areas of science and will benefit from the interaction with other users who come from different subjects. In the heading of each topic we indicate which of the proposed instruments will be mostly used for that particular area of science.

2.3.1 Physics

*Electronic structure - Non-resonant (MIX)*

Non-resonant x-ray experiments can be used to study valence- and weakly-bound-electronic excitations in relatively light materials. These investigations are focused on obtaining a deeper understanding of the band-structure and electron correlation effects. Although soft-XAS is a powerful technique that enables the ground-state local properties to be determined, it is not the best way to determine the energies of the low lying excited electronic states because the energy width is limited by the core-hole lifetime and furthermore energies and intensities can be modified by the core-hole potential. In contrast, if these excitations are measured with IXS, the excitations can be measured without these complications. Non-resonant scattering of x-rays from the relatively low-energy electrons is a rapidly developing and powerful technique for chemistry, physics and materials sciences. It can be used to study K edges of low-Z materials, M edges of transition metals, N edges of rare earths and O edges of actinides. One advantage of the technique is that the scattered intensity can be measured as a function of the wave-vector transfer. At small wave-vectors the scattering is dominated by the electric dipole approximation but at larger wave-vectors the scattering has components arising from higher multipole transitions. Analysis of these intensities enables the $\ell$-projected densities of states to be determined which gives a very stringent test of electronic theories. This type of approach has been demonstrated by measurements on doped superconductors, lanthanides and actinides. These measurements can be readily analyzed because the formalism of the non-resonant scattering cross section is well known and understood.

*Electronic structure - Resonant (SIX, MIX)*

The RIXS instruments are essential for studying fundamental problems of the electronic structure. For example, the types of electronic excitation that can be studied are $d$-$d$ transitions that are not active in either infra-red or optical absorption, and so IXS becomes the preferred technique. These transitions occur when an electron is excited to a higher energy level that forms part of the same electric configuration. They occur in most materials with a partially filled $d$ level. Measurements of the $d$-$d$ transitions for MnO, CoO and NiO have been made in the region of 0.8 to 2.5 eV. Charge-transfer excitations are another example that is difficult to measure with techniques other than IXS. One electron, usually from a partially filled state, transfers to a neighbouring ligand site, and the electron-hole pair then propagates through the sample. IXS techniques enable the dispersion relations to be measured for these charge transfer excitations. High energy crystal-field levels in systems can have both spin and orbital components, the components of which change as the wave vector is altered. These excitations are known as orbitons and have been observed using IXS.

*Magnetic excitations (SIX, MIX)*

Measurements with RIXS enable the magnon dispersion to be measured although the direct coupling between a magnon and the x-rays is very small. A particularly striking example is the measurement of the spin waves in La$_2$CuO$_4$ which is a two-dimensional antiferromagnet with the spin waves increasing in energy up to 320 meV at the zone boundary. The spin waves were first measured with neutron scattering measurements but more recently consistent results have been
obtained with IXS\(^1\) using a resonance appropriate for the \(\text{Cu}^{2+}\) ion. This and similar results show
that magnetic excitations can be measured with x-rays. Thus RIXS offers the possibility to measure
collective magnetic excitations (not just spin waves) in topical correlated electron systems such as
high temperature superconductors and quantum magnets.

**Magnetic scattering and the multipole moments of the ground state (SIX, MIX)**

Another example of the use of RIXS for magnetic systems is in combination with a sum rule
analysis to obtain ground-state information as represented by an expansion in coupled multipoles of
the orbital and spin moments. The experiments are based on the angular dependence of the
integrated peak intensities. In polarized x-ray absorption spectroscopy (XAS) the charge
distribution of the excited core hole is not only characterized by its integral, which is proportional to
the absorption, but also by its spatial distribution, which is in general not spherical. The information
about the deviation from the spherical symmetry, arising from the core-hole polarization, can be
obtained by measuring the angular distribution of the particles emitted by the decay of the core
hole. These particles can either be Auger electrons from the auto-ionization process connected with
the core-hole decay or photons re-emitted by a RIXS process. Since the measured deviation from
the spherical symmetry of the core hole is directly connected with ground-state properties via the
transition matrix elements of the RIXS process, important information about material properties —
not accessible by XMCD in XAS — can be extracted. This additional information can be found in
pure form, if the incident light is perpendicular to the magnetization, in which case the dichroism in
absorption vanishes. In this case we speak of RIXS in a transverse geometry, where the plane
defined by the incident photon and the emitted products detected in the experiment contain the
magnetization direction. The detection of the emitted products breaks the mirror symmetry of the
system, thus providing information about the non-spherical part of the core-hole distribution.
Measurements on Ni and Co ferrite and metals have been made with circularly polarized soft x-rays
at the \(L_{2,3}\) edges and show that the atomic-like properties can be quantitatively obtained up to 4th-
order multipoles.

**Strongly correlated materials (SIX, MIX)**

Resonant scattering has enabled progress to be made for some very complex problems. One of these
is the study of the electronic properties of complex insulators such as Mott insulators. When these
materials are doped they show a variety of different properties such as high temperature
superconductivity, the loss of antiferromagnetic properties and unusual conductivity. The electronic
excitations of some high-temperature superconductors containing \(\text{Cu}^{2+}\) ions have been measured
using x-ray scattering but this is a very difficult field. The results will enable progress to be made in
determining the nature of the pseudo-gap, and by measuring the electronic excitations that cannot
be described by a one-electron picture. An example is the measurement of the electronic energy
levels for YBCO found at energies of around 450 meV where there has been no agreed explanation
for the results\(^2\). There are a large number of materials known that have unusual electronic
properties, in addition to the high temperature \(\text{Cu}^{2+}\) based superconductors, and where x-ray
experiments can play an important role. They include, for example, the Fe based superconductors,
the charge and magnetic excitations in the manganites, the magnetic properties of the Heusler
materials, such as \(\text{Ni}_2\text{MnGa}\) and the effect of doping with Cu, and the topical \(5d\) transition metal
oxide such as iridates which can show topological insulating and magnetically frustrated Kagome
behaviour.

**Phonon spectra (HIX)**


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Measurements can be made for a wide range of materials as shown by the experiments performed at the ESRF. X-ray scattering is particularly suited to experiments with small crystals. Examples are the study of the dispersion relations of novel superconductors such as Fe-pnictides, PuCoGa$_5$, and cobaltilites, where large crystals are rarely available. Another example is the measurement of the dispersion relations for PbMg$_{1/3}$Ta$_{2/3}$O$_3$ which is a relaxor ferroelectric and where large crystals are unobtainable. A slightly different type of experiment is the study of the phonons in materials like carbon nanotubes or the layer material graphene.

**Pressure dependence of phonons and electronic excitations (HIX, MIX)**

The pressure dependence of the phonon spectra can be measured with IXS because the samples can be much smaller than for neutrons. Measurements of the density of states will enable the phase diagram to be determined and any phase transitions to be followed.

### 2.3.2 Materials Science

**Electrons at interfaces (SIX, MIX)**

The small spot size of the incident beam and the selectivity of the RIXS process will enable the properties of the electrons close to interfaces or surfaces to be measured. This will enable devices to be made and to understand their properties in detail. In a similar way, the electronic properties of nanodevices will be determined to find the excitations localised at the boundaries between different materials.

**Phonons in disordered materials (HIX)**

One of the advantages of using x-rays is that the change in the wave-vectors of the incident and scattered beams is very small for significant changes in the energy. The result of this, together with the different kinematics, enables experiments to be performed at small wave-vector transfers for relatively large energy transfers, particularly when compared with similar experiments performed with neutron scattering techniques. X-ray scattering is to be preferred for studying the phonons and other excitations in disordered materials, glasses and liquids. X-ray Raman scattering is also useful to measure the electronic structure which then gives information about the crystallographic structure that can be an important complement to the information obtained from diffraction experiments. This is exemplified by the studies that have been made of liquid water and of ice.

**Functional materials (HIX)**

Experiments will be performed to understand and exploit materials where the lattice, the magnetic and the electronic systems all interact with each other. Often the properties of these systems are finely balanced and can give rise to unexpected behaviour such as the coupling between the electronic and phonon degrees of freedom. These materials may then lead to new functional materials that may have important applications. Examples of these materials are relaxor ferroelectrics, multiferroics, thermoelectrics and superconductors. The ability to study them when an external field is applied, such as an electric current or magnetic field, is the way to understand how these materials behave under real operating conditions.

**Phonons at interfaces and surfaces (HIX)**

The highly focused beam can be used to study exceedingly small samples. This enables the sampling of different parts of a microstructure and hence to improve the performance of micro-
devices. It could also be used to study the behaviour of the phonons at interfaces and surfaces.

2.3.3 Chemistry

Hydrogen storage materials (MIX, HIX)

The storage of hydrogen is a key barrier to the adoption of hydrogen as a clean energy vector. This is a material science problem and a great deal of beam time at facilities around the world is being devoted to understanding the properties of hydrogen storage materials. Inelastic scattering provides information on the bonding of hydrogen, which is a unique measure of a materials kinetics and thermodynamics. Inelastic neutron scattering is a powerful tool and there are many groups using this technique in the UK. However it suffers from poor resolution at high energies and kinematic constraints limit measurements to high momentum transfers. Hydrogen stretch modes and overtones are to be found at energies of several hundred meV where high resolution MIX would make it possible to see the effects of the crystal environment on these modes. Hydrogen recoil at high momentum transfers often smears out the vibrational modes in hydrogen systems, inelastic x-ray scattering will make it possible to measure clean vibrational spectra over a wide range of energies at low-Q where there is little or no recoil.

The science in this field is now moving away from simple one component hydrides to complex heterogeneous materials that are nanostructured and incorporate catalysts. Micron sized x-ray beams will make it possible to study systems that are much closer to application in both fuel cell and hydrogen storage applications.

Catalysis and electrons at surfaces and interfaces (SIX, MIX)

So far we mostly discussed the use of RIXS for determining the properties of bulk systems. There are other important uses for RIXS. One of these is the study of surfaces and interfaces. If these are composed of different elements it is possible to tune the energy to a resonance of the atoms placed on the surface. This then discriminates against the scattering from the substrate so that the surface material can be studied. The electronic structure of the surface material can then be determined and its orientation with respect to the surface. This technique has been used for systems such as a N\(_2\) molecule absorbed on a surface of Ni or carbon monoxide absorbed on a surface of Cu. Clearly these measurements are important for understanding the mechanism of catalysis.

Electrons in nano-systems (SIX, MIX)

This is a similar technique to measure the changes in the electronic structure as the nano-particles are increased or decreased in size. It has been used to determine the electronic structure of cobalt nano-crystals varying in size from 3 - 9 nm and suspended in liquid C\(_6\)H\(_4\)Cl\(_2\). The results show that there is a charge-transfer excitation from the Co particle to the organic solvent which changes as the size of the cobalt particles was increased. Similar experiments can be performed to study oxidation processes such by using an oxygen resonance to obtain the crystallographic and electronic structure of oxygen atoms on say an iron surface. The electronic structure of intercalated materials, such as Er in graphite or CuCl\(_2\) in graphite, can also be studied using resonant x-ray scattering.

Liquid and gas phase vibrational spectroscopy (SIX)

The elemental sensitivity of RIXS along with the high energy resolution offers novel opportunities to measure vibrational spectra of individual functional groups of molecules in liquid as well as in
dense gas environments. This has recently been demonstrated for molecular oxygen\(^3\). It offers a method to study vibrational modes that are not accessible to optical techniques and gives an unambiguous chemical assignment.

### 2.3.4 Earth Sciences

**Mineralogy** (MIX, HIX)

RIXS is the ideal method for determining the oxidation states of natural mineral phases which remain undefined accurately despite considerable investigation. Formal oxidation states are often assigned using XAS or other spectroscopic information but these do not fully explain the fundamental properties of the minerals, their behaviour of the minerals in Earth's complex systems and, in some cases, their response to mineral processing. RIXS provides the opportunity to make major advances in this understanding. The Mineral Sciences communities would benefit greatly from this development.

**Studies of the Earth’s mantle** (MIX, HIX)

To understand the properties of the Earth requires measurements to be made of rocks and other materials under the conditions present at the centre of the earth. This implies performing experiments under high pressure and high temperature and studying the phonon spectra and electronic spectra to determine the phase transitions that occur as the pressure and temperature are both increased.

### 2.3.5 Biological Science

**The bonding of water to biological molecules** (MIX)

Experiments have been performed to study how water is bonded to biomolecules. Experiments were performed using neutron scattering techniques but the resolution was poor especially at large energy transfers. X-ray scattering will be used to obtain better resolution especially for energy transfers between 100 and 600 meV. Furthermore resonant experiments could be performed to try to measure the different ways that the water is bonded.

### 2.4 Existing Inelastic Scattering Beamlines Elsewhere

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<th>Facility</th>
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*Table I: Some details for the inelastic beam lines found at different facilities worldwide.*

The league table of soft x-ray scattering instruments is currently headed by SAXES-ADRESS at the

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SLS \(^4\) closely followed by AXES-ID08 at the ESRF. Both are excellent instruments but we believe to be able to outperform these two instruments. The main advantage will arise from the longer exit arm length (10 m for SIX, as opposed to 5.2 m for SAXES and 2.2 m for AXES) and building a new instrument now enables us to take advantage of the advances that have recently made with the optics. A longer arm will reduce the acceptance angle of the CCD detector and hence the intensity of the scattering but this can be largely recovered by adapting the optics.

The league table of hard x-ray instruments is currently led by ID28 at the ESRF and IXS-CAT at the APS. The ESRF instrument uses crystals with high index planes to obtain the required resolution which inevitably means that the incident energy must be between 20 and 30 keV. The beam intensity at Diamond is decreasing for these energies and so would be unable to fully compete with these instruments. Fortunately a new approach to the optics of this type of instrument is being developed, as described below (HIX). Before this can be assembled into a new instrument further tests and development effort is needed. We consider, however, that the optics will be developed and will enable a world class instrument operating at somewhat lower energies than the existing high performance instruments.

Because inelastic x-ray scattering is a novel and exciting field we are well aware that new instruments are being built and planned at other synchrotron facilities worldwide. There are three inelastic instruments planned at NSLS-II at Brookhaven in the US. New soft x-ray instruments are being built elsewhere, AERHA on the SEXTANTS beamline at SOLEIL in France, one on the UE49-SGM beamline at BESSY II, Helmholf-Zentrum Berlin, and it is planned to upgrade AXES on beamline ID08 at the ESRF to a high resolution spectrometer called ERIXS. We have kept in close contact with the scientists that are building these instruments elsewhere and we will remain in touch with them to see which new optical concepts they develop. We do not see any reason why these x-ray instruments elsewhere would be better than the instruments proposed below.

2.5 The Community using X-Ray Inelastic Scattering

IXS is a field that is rapidly expanding as both synchrotron sources and instrumentation develop. Currently there are relatively few people in the UK who have had experience of using IXS. However, there are many groups of researchers who could naturally use IXS in their research. These include scientists working in the subject areas listed in Sec 2.3. Our approach is to build two state-of-the-art end stations with resolution which exceeds that at currently operating spectrometers. This will allow the UK community to perform the widest possible range of experiments. At present all of the inelastic instruments around the world are in heavy demand and are normally oversubscribed in excess of a factor of 4. We anticipate that in view of the large range of science that can be studied with IXS this will remain the same in the future, especially because this is a strongly growing field. The letters of support which have been received also demonstrate that there are a large number of UK scientists with very different backgrounds who wish to join in IXS experiments.

There is a large UK community that has used inelastic neutron scattering very successfully at ISIS and ILL. INS and IXS are very complementary probes. While INS is a mature technique with a well-understood cross-section, experiments at high energy transfers, $\Delta E > 300$ meV, expose the limitations of current INS techniques. Two examples of communities which would be able to make good use of IXS are those working on (i) strongly correlated electron systems (e.g. superconductors, quantum magnets) and (ii) hydrogen storage materials.

IXS probes both magnetic and electronic excitations. It offers the possibility to study smaller samples of strongly correlated electronic systems and therefore more exotic systems. Thus there is a

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natural user base for IXS with in the strongly correlated electron community.

The interest in hydrogen storage is demonstrated by the fact that approximately 40% of the time for the MAPS neutron spectrometer at ISIS is currently used for measuring the hydrogen vibrations when hydrogen is absorbed by different materials. It is envisaged that the development of facilities for IXS will enable them to obtain additional information about these systems.

2.6 Industrial and Technological Applications

The experience with inelastic neutron scattering is that, while there has been little direct application for inelastic scattering results, industry has welcomed the further knowledge obtained about the elementary excitations of many materials although it has not been closely connected with the measurements. We expect that the relaxation of the constraint on sample size will make the study of excitations more attractive to industry, particularly in collaboration with academic groups.

New materials. One of the most exciting prospects is the possibility of studying the dynamics in novel functional materials of technological importance. As new systems are developed, parametric studies as a function of composition are often required, and it is usually difficult to obtain crystals of a given concentration that are large enough for inelastic neutron scattering. IXS will enable momentum-resolved surveys of these systems for the first time.

Thin films. Some new materials can only be stabilised in thin-film form. The ability to study films brings the study of dynamics closer to applications.

Nanostructures. Most devices are too small for inelastic neutron scattering experiments. Using IXS it will be possible to study excitations in actual devices, and via resonance to focus on individual components in devices.

Spintronics. The Brookhaven Group reported one-unit-cell sensitivity of the resonant scattering technique. This demonstrates the possibility of studying excitations in surfaces and interfaces for magnetic recording devices and magnetic nanostructures in recording media.

Thermoelectrics. The development of high-resolution spectroscopy will enable the study of rattling-mode phonons in new thermoelectric materials that are currently only available as tiny crystals, and these can be used for environmentally friendly Peltier coolers and devices for the conversion of waste heat into useful power. The possibility of studying the dynamics of these systems in thin film and nanostructured form is also exciting, since finite size effects are known to dramatically improve performance.

Multiferroics. The ability of IXS to couple to different degrees of freedom is well matched to the functionality of multiferroics with potential for sensor applications.

Catalysts. The sensitivity to thin surface layers and the ability to discriminate between absorbed molecules and substrates via resonance makes IXS ideal for the study of the dynamics of catalysts.

Hydrogen storage. There is evidence that IXS may be used to study hydrogen vibrations via the effect on the surrounding ions in the lattice. This may open up new opportunities to study the new hydrogen storage materials since, for example, IXS will give access to the high energies of the hydrogen stretching modes.

Carbon-free energy. The high resonant cross-section of the actinides makes them ideal candidates for inelastic x-ray scattering experiments. An understanding of the new materials used in Generation IV reactors is a key ingredient in developing alternatives to fossil fuels.

2.7 Research Councils and Welcome Trust

5 J. Hill, IXS Beamline Workshop, Diamond Light Source, 6th December 2010.
One of the main purposes of the Research Councils and the Welcome Trust is to support world class science to improve our understanding of the natural world. This application provides two new instruments at Diamond that will be comparable to instruments elsewhere in the world and which will be used by a strong and active research community that already exists in the UK. The instruments will be used by scientists coming from the UK Universities and will provide access to world class instruments for the training of their staff and students.

The research councils state that their priority areas in the physical sciences are to study problems associated with sustainable energy, the digital economy and environmental change. IXS will contribute greatly to problems associated with energy by their contribution to understanding the actinides and their waste when used in a reactor system as well as by developing new hydrogen storage materials. The experiments to study functional materials and the experiments on surfaces and interfaces will contribute both to new developments in energy and in the digital economy while the geophysics experiments will contribute to better understanding of the Earth and of environmental change.

3. Beamline Requirements

The beamline requirements are for two separate instruments, each with its own undulator. The first of these, and initially the focus of the project, is a soft x-ray branch (SIX), with a large spectrometer housed in a new external building. The second branch – for hard x-rays – will cater for a variety of experiments, initially RIXS and NrIXS (MIX). This branch will also provide a test facility for the development of a novel millivolt spectrometer (HIX). The hard and soft x-ray branches will be built in separate optics hutchies so that they can operate in parallel and independently.

We propose concentrating effort on the soft x-ray RIXS branch initially, as this is perceived as a very high priority for the user community. It is the largest part of the construction project, and the technical expertise exists to construct an internationally-competitive facility.

The hard x-ray branch will follow, and focus initially on RIXS, but also with a capability for non-resonant scattering. This branch will also support a continuing development programme in novel optics for IXS, with a particular emphasis on new approaches to achieving meV energy resolution with photon energies in the 5-10 keV range. The millivolt spectrometer is the only aspect of the proposal where a technical solution has not been demonstrated, although recent developments at the APS and NSLS have shown very promising results. It is expected that a decision as to when (or whether) to implement a millivolt facility will come later, and will not impact on the requirements for a two-branch beamline. The hard x-ray branch will be designed to be more versatile than the soft x-ray branch, and will be able to take advantage of new developments and new scientific directions.

<table>
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<tr>
<th>Technique</th>
<th>Incident energy (keV)</th>
<th>Energy resolution (meV)</th>
<th>Maximum energy transfer (eV)</th>
<th>Q_{max} (Å⁻¹)</th>
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<tr>
<td>Soft RIXS (SIX)</td>
<td>0.4-2.0</td>
<td>20-50</td>
<td>60</td>
<td>~0.9 (at 0.9 keV)</td>
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<tr>
<td>Hard RIXS (MIX)</td>
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<td>50-150</td>
<td>50</td>
<td>~9 (at 9 keV)</td>
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<tr>
<td>Hard NrIXS (MIX)</td>
<td>5-12</td>
<td>50-150</td>
<td>1000</td>
<td>~9 (at 9 keV)</td>
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<tr>
<td>Hard high-resolution (HIX)</td>
<td>~10</td>
<td>0.4-3</td>
<td>0.2</td>
<td>~9 (at 9 keV)</td>
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</tbody>
</table>

Table II: Estimates of some key parameters for various IXS techniques and proposed spectrometers. Initially the focus will be on SIX and then MIX.
The undulators will be situated in Long Straight 21. A suitable layout for the electron beam optics, to accommodate two undulators in a long straight, has been designed for I13 and I09 – the ‘mini-betap’. We propose essentially the same solution for I21, pending a detailed design study, which will allow a hard x-ray plane undulator, ~2 m long, to be located upstream, and a soft x-ray Apple-II undulator, ~2.6 m long, downstream. Polarization of the hard x-ray beam will be achieved with a diamond phase retarder.

Some of the key parameters and specifications, relevant to the various techniques, are presented in Table II. For these photon-hungry experiments, the most important limiting factor is the incident beam flux. Estimates for these are given in Fig. 2 which suggests the proposed instruments will be comparable with the very best currently available.

![Fig. 2: Calculated photon flux for the soft and hard x-ray undulators at Long Straight 21. As a low-emittance medium-energy source, Diamond undulators are world class in the soft x-ray region (left), and highly competitive up to energies of 10-12 keV, using high-order harmonics (right: 5th, 7th, 9th and 11th harmonics – red lines). Recent developments in undulator technology should provide even higher fluxes (blue lines) in the near future.](image)

### 4. Beamline Specification

#### 4.1 Introduction

The technical solutions proposed here are indicative and represent a ‘baseline’ layout. It is highly likely that some of the features will be replaced or enhanced as technology improves and as new ideas are tested.

The balance between risk and novelty is important to consider. The soft x-ray branch (SIX) proposal is based on an incremental development of a current world-class facility (ADRESS at the SLS) leaving open the possibility of developing an alternative approach if proven advantageous. Similarly, most of the hard x-ray MIX optics is based on existing successful designs. Our proposal for a millivolt non-resonant instrument, HIX, is novel and therefore attracts an element of risk. There are at least two possible solutions that have been identified and are being modelled. Moreover, staff from Diamond is participating closely with a development project based at the APS (under the leadership of Yu Shvyd’ko) that has recently produced some very exciting results. We propose to make the hard x-ray RIXS facility available to users for much of the available time, while testing the optics for a millivolt spectrometer in the remaining time.
4.2 Soft RIXS Branch (SIX)

The soft X-ray RIXS facility will have an energy range of ~400 – 2000 eV (covering the 3d L- and 4f M-edges) and will be based largely on an incremental development of the proven design for the world-leading ADRESS beamline at the SLS. The main optical components of beamline will be a variable-polarization APPLE-II undulator, a collimating mirror, a plane-grating monochromator, a focusing mirror, a microfocus refocusing mirror, and a spectrometer based on a variable-line-spacing spherical-grating analyser, focused onto a tilted CCD detector. The photon flux is expected to be comparable to that of the SLS facility, and we expect improvements of the optics slope errors, CCD technology, and a longer spectrometer arm (10 m), to provide an enhancement of the currently-achieved energy resolution. (We note that higher resolution is achieved at the expense of flux, but a significant increase in the data collection time for such flux-hungry experiments is not considered a viable option).

Unproven alternative designs, whereby the spectrometer is dispersive in both the incident and scattered beam, are of considerable interest as they have the potential to reduce the acquisition time very significantly. This will be modelled in detail as a possible design for Diamond, but the 'baseline' design is based on the more conservative scheme whereby the incident energy is scanned and only the optics for the scattered energy are dispersive.

![Fig. 3: Dispersive analyser for the soft RIXS spectrometer. The source for the spectrometer is the illuminated part of the sample (a few microns in size). A variable line spacing spherical grating focuses light of a particular energy onto an arc across the (inclined) CCD detector, allowing the detector to give very high resolution in energy and wave-vector.](image)

![Fig. 4: Ray-tracing results from the proposed dispersive analyser, based on a 9 m arm. The results show excellent separation of the phonon beams with the mean energy of 930 eV and ±10 meV. The effects of slope errors, the detector point-spread function and the energy bandwidth of the incident beam, are not included but can be compensated for by the use of a slightly longer arm as proposed in this document (10 m). Overall, for the whole instrument, the energy resolution is expected to be no more than 20 meV.](image)

The undulator of choice is likely to be an APPLE-II variable polarization device, of length ~2.6 m, located at the down-stream ID position of a Diamond mini-beta arrangement. It will thus provide linear polarization at arbitrary orientation, as well as left- and right- circular polarization (the latter is likely to be restricted to below ~1.0 keV).

The requirement for rotating the spectrometer arm (about a vertical axis) up to large scattering angles, is important to enable the full range of momentum transfers to be available for the experiments. As with most developments of analyser optics, an obvious direction for enhancement is to construct multiple analysing spectrometers, to be used simultaneously. This will not only improve total data collection rates but also remove the need for very large movements (or possibly...
any movements at all) of the spectrometer arm. These considerations will be considered carefully as part of the technical design.
4.3 Hard X-ray Branch

The hard x-ray branch will operate independently of the soft branch, and provide a number of techniques, characterized by the different requirements for energy, energy resolution and flux. The use of the facility will therefore be determined by future scientific priorities and the available optics. The main uses of the end-station can be split into three main categories: RIXS, NrIXS and ultra-high (meV) resolution. We consider technical solutions for each of these in turn.

4.3.1 Hard X-ray RIXS (MIX)

The resonance provides a large enhancement of the electronic excitation cross-section by tuning the incident beam energy to that of an atomic absorption edge and creating an intermediate state with a core hole. The energy range of interest covers the $K$-edges of the $3d$ transition metals and $L$-edges of the rare-earths, as a primary consideration. In this energy range (~5-12 keV) Diamond undulators perform extremely well, and we expect a 2 m in-vacuum cryogenic device to be comparable to any other third-generation light source.

In the last few years, huge advances have been made in the design of the optics for such instruments, with monochromators based in two- or four-bounce Si crystals (following a high heat-load Si monochromator, see Fig. 6). The analysers are based on the classic spherically-bent design, but recently using relatively large (few mm) flat tiles, while providing a strain-free solution, mounted as close as possible to back-scattering within the constraints of matching the $d$-spacing of a suitable material to the absorption edge energy, together with position sensitive detectors to simultaneously detect spectral components differentially in space. This has been shown to be extremely successful at the APS MERIX beamline, for example. One of the strengths of this approach is that the analysers can cover a relatively large solid angle, i.e. $N$ analysers, each of 100 mm diameter, mounted at ~2 m, where $N \approx 10$. 

Fig. 5: Preliminary layout of the IXS beamline, showing the outline radius of a 10 m spectrometer arm, taking some space that is currently used by peripheral labs and the lawn adjacent to the road. The two undulators are to be located in Long Straight 21, modified to form a 'mini-beta' layout. The new proposed building is seen on the right-hand side, the large semi-circle shows SIX, the small semi-circle shows MIX.
The large angular acceptance of these analysers, combined with the modest energy resolution of ~30-100 meV, provides manageably short data collection times with access to large momentum transfers. Going beyond this energy resolution would require significant loss of flux. The most obvious limitation with this setup is that, while a single medium resolution monochromator can cover the entire energy range of interest, a dedicated set of spherical analysers is needed for each absorption edge.

### 4.3.2 NrIXS Scattering at High Energies

Non-resonant scattering has similar technical requirements to RIXS. Non-resonant IXS measures the dynamical structure factor, \( S(\omega, Q) \), which is easy to interpret, and can be applied to any system. It is easier in the sense that the energy can be chosen arbitrarily and can match the requirements for back scattering. The requirements for Compton scattering are similar, except that there is no benefit in changing the sample scattering angle – backscattering is always preferred.

### 4.3.3 Millivolt spectrometer (HIX)

High-energy third-generation light sources are well matched to the 'classic' single-bounce Bragg back-scattering approach for providing millivolt energy resolution. These spectrometers select a very high order Bragg reflection for both the monochromator and the analyser crystal, requiring energies of ~15-30 keV. This approach has been very successful and the only major problem, other than the high energy, are the long tails of the spectral function arising from the single monochromator or analyser reflection.

In order to construct a competitive facility on a medium energy synchrotron, such as Diamond, an alternative optical design is needed that employs photon energies that are better matched to the
source, i.e. ~6-10 keV. No such scheme has yet been proven. However, there is considerable effort globally in developing millivolt (or sub-millivolt) spectrometers for medium energy sources. Perhaps the most promising of these is the CDW (collimating/dispersing/wavelength-selecting) design of Yuri Shvyd’ko from the APS (Fig. 8). Diamond staff has been involved in a collaborative effort to prove this technology, and have very recently -- and successfully -- tested a novel collimating optic (Montel mirror with variable period multilayer coating, see Fig. 9) that will reduce the divergence of the beam from the sample sufficiently to allow a CDW analyser. Recent preliminary results from the APS are also extremely encouraging, giving a measured efficiency of the CDW monochromator of 16% at 0.42 meV resolution – getting close to the theoretical value of 32%. The design is technically demanding but has the potential to give sub-meV resolution at medium energies, with a solid angle essentially the same as with the backscattering geometry. More testing is needed before a complete instrument can be constructed, but this remains one of the most promising technologies for a millivolt spectrometer, as an upgrade for the IXS hard x-ray branch.

Fig. 8: A possible layout for a HIX spectrometer based on the CDW monochromator system under development at APS in collaboration with Diamond Light Source. The CDW monochromator was recently tested very successfully, giving an energy resolution of 0.42 meV.

Fig. 9: The Montel variable-spacing multilayer collimator developed at Diamond as part of the CDW development, shown mounted on the APS MERIX spectrometer. Recent tests at Diamond were extremely encouraging and showed that the performance of the optic exceeded specifications.

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An alternative design, in use for nuclear resonant scattering, is a variation on the four-bounce asymmetric monochromator designed by Tom Toellner (also from the APS) – Fig. 6. This design is unlikely to give sub-millivolt resolution for medium photon energy, but can give around one meV or slightly higher. Moreover, the Diamond Montel collimator may be used in conjunction with a second monochromator as an analyser. Both of these schemes are expected to give very weak tails compared to backscattering analysers, but both need further development. The Toellner design should allow the incident energy to be chosen relatively freely (prior to the manufacture of the optics) and could be chosen to match an absorption edge, such as the Fe K edge. This would give a unique opportunity to measure RIXS with millivolt resolution, albeit at very low count rates compared to the conventional medium-resolution design. Continued development of a millivolt spectrometer is expected to take place during the construction of the IXS beamline, and possibly continue on the beamline as a development project until a suitable solution is obtained.

4.3.4 Sample Environments

Sample environments are the key to extending the scope of a facility for addressing important scientific questions. These are necessarily limited on the soft x-ray branch, due to the strong attenuation of the beam by almost any solid that could be used as a window. A top-loading superconducting magnet/cryostat would be extremely useful and would fit well into the overall geometry of the instrument. A detailed analysis of the technical considerations of such a device (e.g. the implications for non-magnetic components) will be given at the design review stage. Sample environments for the hard x-ray branch are less restrictive and should include capabilities for high pressure (specially designed DAC), low and high temperatures and a magnetic field.

5. Costs and Staffing

The proposed beamline comprises two independent end-stations, and external building and very advanced optics. The most accurate estimate of the cost is likely to be very close to that of a similarly complex two-branch (hard and soft) beamline currently under construction, plus the cost of a comparable external building. The most relevant comparisons are I09 (SISA) which has hard and soft x-ray undulators, one optics and two experimental hutches. The cost of the beamline, including a hemispherical electron analyser system of comparable value to an x-ray spectrometer, is xxx. Estimates for the front end and undulators are xxx and 2 xxxx. The other major expense is the external building. This is comparable to that of I12 but slightly larger and the estimated cost has been scaled with the increased width to give a figure of xxx The relative complexity of the I12 building is lightly to compensate largely for the cost of the spectrometers. The on-going development of optics and spectrometers, especially for the HIX project, will require further staged funding. We estimate that £xxx will be required over a period of two years after completion of the beamline including SIX and MIX facilities. The total budget estimate is therefore:

Main beamline (with SIX and MIX facilities): £xxx
Phase-II development (largely HIX): £xxx

The above figures are based on the assumption that the hard and soft x-ray branches are constructed simultaneously, which would prevent the construction of one branch impacting on the use of the other. If staged construction is required then initial emphasis would be on the soft x-ray facility (SIX). The initial cost saving would need to be looked at in detail but is unlikely to be more than about 25% without seriously compromising the operation of the SIX instrument.

Staffing costs will reflect the fact that there will be two independent end-stations, operating in
parallel. This will ultimately require twice the number of scientific and technical staff as a single beamline, plus continuing input from the Diamond optics group for R&D.

Summary of Beamline Specification

The current proposal is for two end-stations on an I21 mini-beta layout. The first is a large soft x-ray spectrometer (SIX), radius up to 10 m, located in an external building, and using an APPLE-II soft x-ray undulator. A hard x-ray undulator will supply a second end-station, located in the main building. The latter will provide a hard x-ray medium resolution RIXS facility, similar to the APS MERIX beamline (Figs. 6 and 7), named MIX, which will also be suitable for non-resonant scattering measurements. The hard x-ray end-station will also be used for the development and testing of novel optics towards the construction of a medium energy millivolt spectrometer (HIX) which it is hoped will eventually provide a competitive high resolution IXS facility and also allow users to broaden their span of research activities.

6. Letters of Support Table

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<th>Institution</th>
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<td>Cavendish Lab, University of Cambridge, UK</td>
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<td>Radaelli, Prof Paolo G.</td>
<td>Clarendon Lab, University of Oxford, UK</td>
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<td>Roberts, Prof Kevin J.</td>
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<td>Aberystwyth University, Wales, UK</td>
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