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Diamond Beamline C

A Core X-Ray Spectroscopy Beamline (EXAFS)

A proposal prepared for the SAC May 2002

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Beamline C

A Core X-Ray Spectroscopy Beamline (EXAFS)

1. Summary

It is proposed to build a high performance X-ray absorption spectroscopy beamline on a bending magnet source at Diamond. The beamline will support a wide and multidisciplinary research programme.

XAS is an established technique that exploits the intense and continuous radiation emitted by a bending magnet or a wiggler source on a synchrotron. With advanced data analysis procedures, many of which have been developed in the UK, XAS routinely provides essential information about the local atomic geometry and of the chemical state of the absorbing atom. It is element specific and is not restricted to the crystalline phase, but may be used with highly disordered amorphous and liquid samples. The power and versatility of the technique has meant that XAS is the preferred experimental tool for many non-specialist users and is an essential facility on all medium and high energy light sources.

This will be the first general purpose XAS beamline on Diamond. It will be used for an extensive range of studies that will underpin research programmes supported by all the funding agencies. More than thirty researchers have expressed support for the beamline. Proposed research includes measurements of semiconductors, materials at high pressures, phosphate and silicate glasses, ion conducting solids, catalysts and microporous solids, hydrothermal reactions and reactions at the surfaces of minerals. XAS is an essential tool for environmental science. It is needed to identify dilute quantities of toxic metals in the soil and to develop methods of arresting their flow into water supplies. XAS has application to bio-active materials and for the study of transitions in metallo-proteins.

By building the beamline to the highest standards of data collection and optical quality, it will be in demand for reference measurements in metrology, patent definition and forensic science.

2. Scientific Requirements

During the past twenty years X-ray absorption spectroscopy has developed from a technique practised only by specialists to a tool accessible for ‘one time’ users. This increase in reliability has emerged from an improved understanding of all parts of the optical system, the detectors, data acquisition and analysis. Agreement upon the best procedure for data analysis is emerging.
However, the validity of the final results still rests upon the quality of the experiment. One objective of the core beamline is to make the highest current standards of data collection in XAS the norm for experiments on Diamond. The beamline will be developed to offer a high spectral purity, the lowest possible noise levels and the energy of the scans should be calibrated to traceable standards. This will permit the beamline to be used for important reference studies not only in metrology, but also in patent cases and forensic science. Furthermore some examples of the wide areas of science in which the core beamline will be employed are given in the following sections.

2.1 Physics of materials and metrology of XAS

Semiconductor physics

The diminishing size of semiconductor devices makes the use of diffraction techniques harder, and the use of XAS more attractive. Work is progressing on the development of nanocrystalline InN and InGaN materials for optoelectronic applications. The materials are only a few monolayers thick, making REFLEXAFS an ideal technique for studying the relationship between local structure and function.

High pressure condensed matter

High-pressure physics has made enormous advances through use of SR techniques. Most studies have involved diffraction, but in comparison there have been few combined XAS / XRD studies at high pressure. There is considerable interest in the structure of high pressure melts, not least because understanding of these is required to explain the evolution of the earth’s core and its magnetic field. High-pressure studies continue to provide the data for development of accurate interatomic potentials. High accuracy variable temperature XAS studies will be used to improve understanding of thermal factors in XAS analysis.

2.2 Chemistry and Materials

X-ray absorption spectroscopy is a prime tool in the field of materials science and chemistry, since it is the only technique that offers element-specific structural analysis under non-vacuum conditions. X-ray spectroscopy is often the technique of first choice for structural studies of complex disordered materials. It is frequently the case that the chemistry of the minority component determines the properties of the whole system. Good examples are to be found in materials chemistry, analytical chemistry, corrosion science, heterogeneous and homogeneous catalysis and process optimisation. The range of possible applications is enormous. The scope of UK science is illustrated by the selection of examples given below.

Ion conducting oxides, batteries and fuel cells

Solid oxides are a group of materials with very important properties such as superconductivity, ion conductivity and magnetoresistance.

The main interest in oxide ion conducting systems stems from their application as electrolytes in fuel cells, oxygen pumps and gas sensors. This work has predominantly involved studies on fluorite related systems, in particular the stabilised zirconias, which show high conductivities in the order of 10^{-1} S cm^{-1} at temperatures around 1000 °C, but there are exciting possibilities in the study of many alternate systems such as doped bismuth vanadates, perovskites and lithium manganates.

Development of oxide materials for fuel cell application has often been empirical especially in relation to interfacial issues. XAS aids deconvolution of redox processes occurring within specific components of the fuel cells in order to gain a fundamental understanding of the mechanisms of transport across such interfaces. The materials are typically complex, multi-component, oxide ceramics with operating conditions in excess of 500 °C and in various oxidising or reducing gases. Combined XAS/XRD is ideal since it is the short-range structure that is of most importance, in relation to ionic conduction in solids and this is frequently very different from the average structures, especially in the most exciting materials for fuel cell and battery applications.

Fuel cell electrocatalysts are frequently based upon Pt particles supported on carbon. The future value of combined XAS / XRD studies lies in the opportunity to study complete working systems, through all stages of the life of the fuel cell. Conventional XAS studies of battery components (electrodes, electrolytes and interfaces) have played an important role in understanding and optimising materials. This role will continue and in-situ XAS studies of the processes that occur during battery cycling will give very important information on insertion chemistry on battery electrodes, such as those based on tin oxide, in terms of the nature of the alloys formed. The time resolution offered by the core beamline is a good match to the electrochemical procedures used in fuel cell and battery applications.

Materials and Chemistry

XAS is proving an invaluable tool in the development of novel inorganic pigments; materials that have hitherto been discovered by chance or empirical experimentation. Recent work has shown how chromophores are substituted into a host lattice. Depending upon the preparation procedure, dopants may substitute for host lattice atoms or form encapsulated nanoscopic clusters. This can only be determined by using XAS because the loading is too low for XRD. This work will have a considerable impact upon the continued competitiveness of the UK pigment industry.

There is much interest in the discovery of improved materials for application in optoelectronics. There is an enormous range of different materials under investigation a key feature of which is control of optical properties by low levels of dopants (~0.1 atom percent). These materials include phosphate glasses for non-linear optics, doped silicas produced from sol gel processes for application as coatings, filters and ultra-low expansion materials. The objective is the detailed nature of the metal site – a task for which XAS is uniquely suited.

It is likely that bioactive materials will be the highlight of the next decade. Novel biocompatible materials are required for dentition, bone regeneration / replacement and other prosthetic materials. These will be complex materials, possibly derived from amorphous or sol-gel precursors. XAS in combination with SAXS / WAXS will be an important technique for successful developments in this area. Even materials as traditional as leather can benefit from investigation by XAS. The role of Cr (III) in the tanning process is not fully understood and there is a need to develop new and more environmentally benign tanning processes.

It may seem surprising and is certainly not a very popular fact to proclaim, but interesting compounds and materials are still made that obdurately refuse to crystallise or even dissolve in solvents. For these materials, standard or routine XAS may offer the best chance of deducing the structure. An automated XAS system could revolutionise study of this type of material, and be of disproportionately large value to a wide community of chemists and material scientists.

Another area where XAS has made a very significant contribution, as it is the only method of obtaining direct structural data, is the study of highly reactive and unstable species stabilised in cryogenic solids such as argon at *ca*. 10 K. Such information, when combined with other experimental data and high level calculations provides great insight into geometric and electronic structures and bonding. As the ‘samples’ have to be prepared in-situ on the beamline, on-line monitoring using simultaneous FTIR has been developed, and this would be continued on beamline C and expanded to include UV-Vis and possibly Raman. Areas of interest include 3d transition metal halide carbonyl and ethylene complexes, pnictide atom cryochemistry and 4d and 5d precious metal monomeric halides.

Catalysis and microporous solids

X-ray absorption spectroscopy has been invaluable in the determination of atomic architecture of many catalytic systems. A complete list of activity could not be listed here, so a few illustrative areas will be described.

There is a substantial activity in the UK in the area of open framework solids undertaken by a number of world class groups. Open framework solids include micro- and mesoporous silicates, aluminosilicates (zeolites), aluminophosphates and metal ions substituted variants. Interest in these materials stems from their unique adsorption and catalytic properties. X-ray diffraction is used mostly to identify phases and determine the framework structure of these crystalline solids, but X-ray absorption is essential in the majority of the cases, since the catalytic sites generated due to the presence of metal ions (also called heteroatoms) are invariably present in low concentrations and thus substitute at random. In many instances XAS studies alone have been sufficient to determine the structure of the active sites. A highlight of current work is the use of combined studies of the synthesis of microporous materials; the aim of which is to move towards rational synthesis of novel materials.

There remains much to be learnt in many homogenous catalysts. The objective is to study catalysts under working conditions, which includes selecting the normal working catalyst concentration. This can present a severe challenge to XAS, and may necessitate experiments upon a beamline optimised for ultra-dilute spectroscopy. However much can be achieved on the core beamline if it is designed as a low noise station. Systems of interest include catalysts for polymer recycling, alkane hydrogenolysis, and electron transfer reactions.

Ionic liquids are proving to be versatile solvents for a wide variety of processes and XAS studies have shown that dissolution of a number of metal-containing salts and complexes lead to the formation of highly stable small metal nanoclusters. Considerable opportunities exist for in-situ and combined technique studies, because of the very unusual short-range liquid structure.

There is pressure to design catalysts for small-scale high value synthetic processes. Development of small scale multiple reaction cells coupled with online chemical characterisation and automated data collection could reduce both the optimisation time and costs for this type of application.

There is a continuing demand for more efficient and more environmentally friendly catalysts, XAS will continue to play a pivotal role in understanding the relationship between local structure and functionality.

Combinatorial Chemistry

Competition within the chemicals industry is providing a substantial incentive to shorten the time required introducing new processes. The optimisation of chemical processing involves the testing of many catalyst formulations. Use of modern robotics and information processing offers an opportunity to develop a combinatorial chemistry facility at Diamond. Arrays of catalysts are currently screened by such properties as exothermicity, colorimetric response and mass spectrometric signal. This could be extended on the core beamline to include in-situ structural analysis of identified leads. This could greatly enhance both testing efficiency and chemical understanding.

Hydrothermal reactions of industrial materials

At their best X-ray spectroscopy and X-ray diffraction provide essential and complementary information about the structure of materials. One of the best examples of this is in the study of hydrothermal synthesis, where is it possible to study the genesis and transformation of complex multiphase materials on a variety of length scales. This is a well-established methodology in the area of combined techniques. Iron oxide is a very pertinent example of a hydrothermal system of relevance to both earth scientists and chemists. The core beamline will be designed to be compatible with a range of different combined techniques and will improve our understanding of systems as diverse as microwave acceleration of reaction processes and laser heated levitated high temperature glasses and liquids.

Interfacial and surface science

The metal-environment interface is of fundamental importance in a wide range of areas that included corrosion, catalysis, electro-deposition, and biomineralisation. XAS offers the opportunity to probe this interface in-situ allowing a direct correlation between interface behaviour and applied conditions. The core beamline will permit measurements of metal oxidation / passivation; dissolution or leaching of individual components and surface adsorption. Whilst monolayer sensitivity will be feasible, time resolved measurements will require access to a beamline optimised for high flux /ultra dilute. (There is also interfacial aspects in the electrochemistry section, and biomaterials in the Chemistry & Materials section)

Nanoscale Science

There is intense interest in the preparation and properties of materials with nano-sized dimensions. Techniques are now available for the sample preparation of most material types, e.g. metals, oxides, semiconductors, polymers, etc., with particle sizes in the nanometre regime. Many groups are developing techniques to prepare clusters and wires of controlled size and morphology for a variety of applications in nano-electronics, optics and catalysis, which can involve complex phase structures, e.g. quantum dots confined in inert matrices, metal clusters inside porous structures. One objective of characterisation is to determine the structure, interatomic distances, and the mean oxidation state of atoms in the nanoparticle. Combined XAS / XRD has much to offer in this area and will be particularly useful for mixed nanomaterials and confined nanoparticles, where phase separation, alloy core shell structure, and interaction with the matrix can be readily detectable.

Industrial Collaboration

XAS has long been recognised as invaluable tool for problems faced by the chemicals industry. The core beamline will continue a tradition of providing an interface between industry and SR users, so that the most appropriate technique may be selected to tackle problems. These will include the use of XAS to study promoters and poisons in homogeneous and heterogeneous catalysis, and the study of scale inhibitors used in oil production.

2.3 Environmental and Earth Sciences

Environmental

A legacy of Britain's industrial past is large areas of contaminated landscape that present both a health hazard and an inhibition to the productive use of the land. Contamination of the environment continues, an inevitable consequence of industrial and domestic processes, with the containment and environmental impact of wastes, including nuclear wastes, a particular problem. XAS is proving an extremely important tool in identifying the nature of toxic metals causing the contamination and, thus, allowing remediation strategies to be devised. Critical information provided by XAS is the speciation of the metals (solids and fluids) and the role of sorption on mineral surfaces in the cycling of the metals; these factors control toxicity, mobility and bioavailabilty. XAS has provided, and will continue to provide, information on 'heavy' metals such as Cd, Hg, As, Sb, Cu, Zn, Cr and Pb, all products of industrial processes. There will also be a particular future focus on radio-elements in the environment such as Tc, Pu, Np and U as an there is an existing legacy of contamination and waste, and the debate on the future use on nuclear energy has been revitalised. XAS will be used in the study of 'natural' systems and experimental studies, often being the only technique of capable of providing structural information on the non-crystalline components. The results will be transferable to environmental problems across the globe. Illustrative examples are given below:

Arsenic is one of the most prevalent causes of water contamination in developing and developed countries and consequently is stimulating much research into the biogeochemistry of this exotoxic element. The geochemical behaviour of As is governed predominantly by adsorption onto Fe oxyhydroxides. XAS is ideal for determining the oxidation state and local chemical environment of adsorbed As. Insights derived from application of this technique will play an important role in understanding the mechanisms whereby As is mobilised, transported and immobilised in groundwaters and the development of strategies to provide safe drinking water.

Uranium contamination has a dramatic impact on all aspects of the natural environment. Despite this, the levels of U in many surface and subsurface environments remains significantly above background and there is increasing pressure to understand, and predict, the mobility and geochemical cycling of U within the geosphere. To understand and predict U behaviour in the environment it is imperative that we possess knowledge of the behaviour and speciation of U along with the thermodynamic properties of these U species. High quality XAS is capable of providing information on the coordination number, and metal-ligand distances, it may also provide/give evidence for the formation of polynuclear uranium species. This is valuable data for building a model for U transport in the geosphere.

Since the phosphates of many toxic metals are very insoluble, it has been proposed to use bonemeal as a sustainable source of phosphate for remediating soils. The core beamline can make a substantial contribution, by providing high quality XAS data on the bulk composition of soils. Levels of contamination are challenging (ca 50-100 ppm) but feasible. Time resolved studies of simulated soil systems will improve our understanding of nucleation, transformation and ageing of phosphate deposits.

Earth Sciences

XAS is being used to study both the bulk and surface chemistry of rock-forming and economically important minerals. The element specific property of XAS allows mineralogists to investigate the most chemically complex materials including those with only short-range order. Environmental mineralogists are particularly interested in the study of sorption/desorption reactions on the surfaces of common silicate minerals and their role in the cycling of metals. XAS can provide unique information on the structure and structural development of amorphous phases that are known form crucial reactive stages in the cycling of elements at the Earth's surface. Successful studies on Cu, Hg and Fe sulfides will be extended to other sulfide systems, focussing on the inorganic - organic interface and biogenically produced sulfides.

These environmentally relevant studies are being extended to examine surface reactions during mineral processing, especially froth flotation - this understanding will allow improvements in processing efficiency, extending our resources and reducing environmental impact.

XAS has allowed major advances in the understanding the structure of complex minerals by determining the co-ordination environment of individual elements. This has been especially important in solving previously intractable problems in solid solution series and in the study of trace element substitutions - the structural information has helped explain the properties of the bulk minerals (reactivity in nature, magnetic, conductance) and XAS has become an essential pillar of such research. Combined with X-ray diffraction, the short and long range of minerals can be defined. The advances in understanding the XANES of XAS spectra will make XAS an even more powerful tool for the mineralogists in the future.

2.4 Biological Science

The study of biological systems by x-ray spectroscopy presents enormous challenges. Until recently only small amounts of metallo-proteins have been available and the concentration of metal has been so low that very long data acquisition times have been required. For routine structural analysis, XAS cannot compete with PX. On the other hand if the material is partially ordered, the oxidation state in doubt or if there is a need to study a transformation process, then X-ray spectroscopy may be the best if not only means of gaining understanding. Many of the applications foreseen for Diamond will require a high-flux station designed for ultra dilute systems, but extrapolating from current work there will be a steady demand for access to the core beamline for those cases where proteins can be produced in reasonable quantities as result of the structural genomics programmes, for mutant proteins (both natural and laboratory derived) and for ligand binding. A typical application is the study of metal-based therapeutic agents. These include anticancer (Pt), antiulcer (Bi), neuronal (Mn) and antiarthritic (Au) drugs. Of particular interest is the manner in which these agents are transported in biological systems to the site of action. Adducts of these agents with proteins such as transferrin will be eminently suitable for study on the core beamline.

Recent work has shown that in more concentrated systems such as in the malaria pigment, it is feasible to follow bio-inorganic transformations via combined XAS / XRD, so that evolution of short and long range order may be followed in-situ and in real time. Preliminary work of this nature could be carried out on beamline C, in preparation for microfocus studies on single cells using beamline 13, or a station optimised for ultradilute spectroscopy.

Within the radiography community, there is growing interest in the use of synchrotron radiation for X-ray fluorescence studies of healthy and diseased tissues. Recent work has shown much higher sensitivity and better statistics can be obtained from a XAS facility compared to a typical medical or laboratory XRF instrument. The objective of this work is to offer *in vitro* XRF methodology as a support modality in the early diagnosis of breast tissue. The work requires rapid tunability and energy resolving detectors, together with a low fluorescence background. These features should all be provided by Beamline C. This work also maps onto the approved microfocus beamline 13 – ultimately mapping the elemental distribution in the healthy and diseased tissues (with micron resolution) is planned, in order to determine the location of the metals and understand the reason for elevated levels of certain metals in diseased tissues.

3. Beamline Requirements

The scientific case above has been written for a bending magnet source.

Source: Dipole

Optics: Plane 1st mirror coated with 2 stripes of Pt and Rh and blank Si stripe set at 2 mrad vertically, accepting 3mrad horz.

Energy range		2-35 keV;
Resolution ΔE/E		1×10^{-5} to 1×10^{-3}
Photon flux with Si (111) at 10keV:		
	Horz focusing	$3x10^{12}$ s^{-1} (16.5 10^{12})
	No horz focusing	$3x10^{11}$ s^{-1} (BM29 10^{11})
Beam size		
	Focused	~15μm (v)×1mm(h) FWHM
	Unfocused	1mm (v) x 10mm (h)

Water-cooled QEXAFS double crystal monochromator with interchangeable crystals.

Horizontal focusing will be required by either a sagittal monochromator or toroidal mirror

Removable plane or toroidal mirror

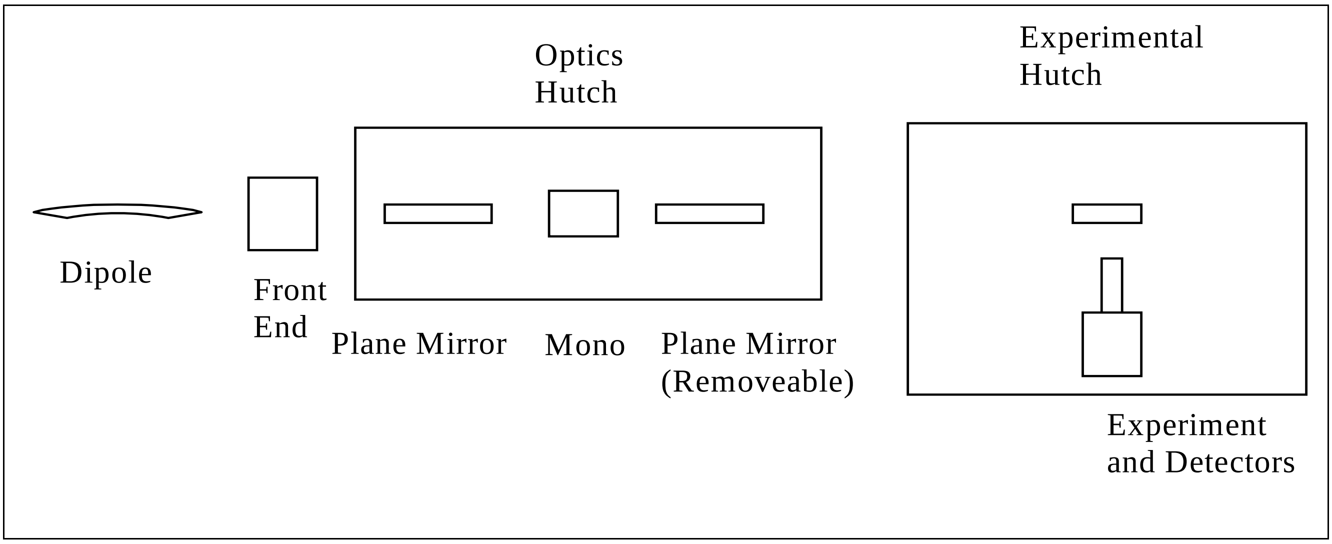
Detectors: Photodiodes, ion chambers, multielement compact solid state detector
Curved gas μ-strip detector for X-ray Diffraction

Software: Flexible environment allowing for easy integration of user equipment, automation of tasks and setting-up, control of multiple techniques and remote access for monitoring.

Sample Environments: Cryostat, furnaces, automatic sample changer – all fully integrated into the data acquisition system. Offline facilities such as sample preparation and chemistry labs are essential.

4. Beamline Specification

The goal is photon-statistics limited performance. Very careful consideration will be given to all sources of noise – mechanical, electrical, thermal, and optical, based upon many years of experience at the SRS and BM29. In order to make the maximum use of the flux, a plane first optic mirror and sagittal focusing monochromator are specified, although a flat monochromator and toroidal 2nd mirror could also be used to focus the beam for a reduced energy range. The first mirror will be set at the same angle as XAS_2a (MPW beamline) for compatibility, but a third uncoated stripe will allow soft edges down to 2keV to be explored. This will limit the upper energy range to about 35keV, above which the flux falls significantly and thus higher edges such as the K edges of lanthanides should be collected on BM29 at the ESRF. Several interchangeable crystal sets will be employed in order to cover the whole energy range with the required energy resolution. The beamline will be built with a large amount of flexibility in order that many different types of experiments can be carried out, but also will have a basic setup (maybe without horizontal focusing) where routine samples can be scanned rapidly via an automatic sample chamber. Thus the beamline will be designed to be easy to set up for simple experiments and for inexperienced users, but flexible enough to allow preliminary or exploratory complex experiments destined for the MPW or microfocus lines to be investigated. It is thus important that the sample area shares a common sample bench with the microfocus, MPW and possibly other beamlines. Provision will be made for rapid interchange of user-supplied environments for complex experiments (high pressure, in-situ catalysis, fuel cells, and corrosion etc). Many experiments will require simultaneous XRD. The detector currently specified is a gas microstrip, but by the time of start-up silicon microstrip detectors should be available.



5. Costs

Front End	
Optics Hutch	
Mirror mechanisms & vessels	
Monochromator	
Slits	
Vacuum equipment and controls	
Hutch & Services	
Experiment Hutch	
Photodiodes, ion chambers & electronics	
Slits	
Sample alignment stages	
Multiple Element compact SSD	
Goniometer for combined and reflexafs	
CCD area detector for combined	
Gas μ-strip detector for combined XRD	
Sample cells, furnaces etc	
Vacuum enclosure & manipulator for light elements	
Optical bench	
Hutch	
Control Cabin	
DAQ computers & electronics	
Temperature controlled Cabin	
Beamline Mechanical Services	
Beamline Electrical Services	
Personnel Safety System	
Beamline Controls	
OffLine Facilities	
Chemistry Labs	
UV-vis Spectrometer	
Total	

Expressions of interest are invited from research groups in using a general-purpose x-ray absorption spectroscopy beamline for the study of materials on the **diamond** light source.

diamond http://www.diamond.ac.uk/ will be built at the Rutherford Appleton Laboratory and is due to be available to users in September 2006. With 24 cells, and at 3.0 GeV, it will be will be unique among the medium energy synchrotron radiation sources and will present great opportunities for fundamental and applied research in both the physical and the life sciences. It will provide very bright radiation from undulators up to 20keV and high flux from multipole wigglers and wavelength shifters to energies greater than 100keV. Bending magnet sources will provide intense radiation over a wide spectral region from 35 keV to the IR.

After consultation with the Science Advisory Committee we are proceeding with the preparation of detailed proposals for six beamlines for consideration for the second year of operation, that is, from September 2007. It is proposed that one of these should be a beamline on a bending magnet for the study of materials using X-ray absorption spectroscopy. The beamline will be for designed for high reliability and accuracy with the minimum of noise background. It will be easy to set up and there will be provision for rapid interchange of user-supplied environmental systems for specific experiments. The outline specification of the beamline is set out below.

Optics: removable plane Si mirror with stripes of Pt and Rh accepting 3 mrad (h);
cooled double crystal monochromator with sagittal focusing giving:

Energy range	2-35 keV;
Resolution ΔE/E	1×10^{-5} to 1×10^{-3} ;
Photon flux:	3×10^{12} s^{-1} in 0.1% bandwidth at 10 keV with sagittal focusing; 1.2×10^{10} s^{-1} at 35 keV with sagittal focusing and mirror out;
Image size	1 mm (v)×10 mm (h) unfocussed, 15 μm(v)×1500μm(h) with focussing.

Detectors: multielement compact solid state detectors
curved gas μ-strip detector for X-ray diffraction

Sample Environment: cryostat (10 K), furnaces.

Expressions of interest, not longer than two sides of A4 should be sent as a word document to diamond@rl.ac.uk by **February 20th 2002**. They should be marked: **BEAMLINE C** and include:

Your name and affiliation;
The overall objectives of your proposed research;
The likely long-term impact on science and technology
And your comments on the outline beamline specifications.

The information will be used in the preparing the case for the beamline and defining its primary aims.

Chris Dobson and Colin Norris
Interim Science Directors for **diamond**

Names	**Affiliations**	**Areas of Interest / Techniques**
Abrahams	Queen Mary College, London	Characterise dopant environments, especially where the dopant is located on the same crystallographic site as the host metal.
Benfield	University of Kent	Study a range of novel nanowire and cluster materials of metals including gold, silver, palladium and iron.
Chadwick	University of Kent	Research aimed at understanding the relationships between point defect structures and atomic migration in solids. A focus is the study of oxide materials with interesting technological applications.
Couves	BP, Research Dept	To study, determine the structure and mechanism of operation of scale inhibitors used in oil well produced.
Covington	University College Northampton	The nature of complexation between chromium (III) and collagen carboxylate, with regard to the degree crosslinking.
Dann	Loughborough University	Studying the local structure of zeolitic materials with unusual framework compositions, which show unusual ordering behaviour.
Evans	University of Southampton	Oxide supported metal catalysts, homogeneous transition element catalysts, and primary steps in metallorganic chemistry.
Farquharson	City University London	X-ray Fluorescence as a Probe in Pathological Breast Tissue.
Flavell	UMIST	Electronic structure studies of catalytically active complex oxides.
Harrison	University of Edinburgh	To follow the hydrothermal growth of metal oxide particles by SAXS/WAXS and XAS measurements *in situ* and the progress of solid-state processes heated by microwave radiation.
Harvey	Daresbury Laboratory	Determination of metal oxidation state and types and numbers of coordinated ligands of the malaria pigment, β-hematin and related systems.
Hardacre	The Queen’s University of Belfast	EXAFS and XANES would be used to characterise a range of heterogeneous samples in an *ex-situ* environment. A wide variety of reactions are studied from environmental catalysis to fine chemical synthesis.
Henderson	University of Manchester	Molecular scale investigations of a range of natural materials, including minerals, soils, colloids, waters, and plant and animal matter and 'contaminants' introduced by human activity.
Irvine	St Andrews University	Intrinsic nanodomain formation in zirconia fluorite’s.
Joyner	Nottingham Trent University	Investigation of activation and deactivation behaviour of heterogenous catalyst as well as the reaction mechanisms of catalysed reactions.
Jones	Keele University	Identify different modes of incorporation of chromphore centres into commercial Zircon based inorganic pigments which have prepared by both conventional and sol-gel routes.
Kilner	Imperial College London	Electrochemical interfaces in Materials Science e.g. fuel cell technology, corrosion, catalysis and biomineralisation.
Murphy	Daresbury Laboratory	Study metalloproteins (both native and site directed mutants) under a wide range of conditions e.g. oxidised,

		reduced, with substrates or inhibitors or with variation of pH.
Newport	University of Kent	Sol gel materials, and in particular those containing metals. Ultra-low expansion materials, filters, dielectrics, Ta, Zr, Hf,Ti.
O'Donnell	University of Strathclyde	Exploring the nanostructure of InN and InGaN epilayers by means of Extended X-ray Absorption Fine Structure (EXAFS) measurements of the indium K-edge.
Parkin	University College, London	Studies into the composition of amorphous alloys and molecular environment.
Pettifer	University of Warwick	
Russell	University of Southampton	Processes of adhesion, corrosion, catalysis, and electrochemistry. The relationship between the structures present at this interface and its properties.
Sankar	The Royal Institution of GB	Determination of structure of heterogeneous catalytic materials, using combined experimental and molecular modelling techniques to derive structure-property relationship enabling the design of new catalytic materials.
Sadler	University of Edinburgh	Determination of metal oxidation state and types and numbers of coordinated ligands in adducts of metal therapeutic agents with proteins and DNA.
Sapelkin	De Montford University	Interatomic interactions under high pressure.
Schofield	Natural History Museum	Establish the speciation of U (VI) in aqueous solutions as a function of pH, temperature, ligand type, and uranium/ligand concentration, using X-ray absorption spectroscopy.
Slater	The University of Surrey	Research on the structure and properties of inorganic solids. New materials for solid oxide fuel cells and novel inorganic oxide fluorides and oxide carbonates.
Walton	University of Exeter	Properties of inorganic solids to optimise their practical application.
Weller	Southampton University	Synthesise new materials, to study their structures and to investigate their physical properties (magnetic, optical and electronic), in relation to the determined structural features.
Went	University of Kent	Determine the structure of transition metal complexes, and use this information in the design of potential radiopharmaceuticals.
Wright	St. Andrews University	Study the local environment and oxidation state of transition metals and metal oxides within porous solids.
Young	The University of Hull	Investigating the structure, reactivity and bonding of small vapour phase inorganic compounds.