New Scientific Opportunities at the European Synchrotron Radiation Facility

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1. Introduction

The ESRF's 6 GeV storage-ring light source, built in the early nineties, is the first insertion device based ("third generation") synchrotron radiation (SR) source. The ESRF has been extremely successful, in terms of both technical innovation and a very large volume of new and exciting science. With some 5500 scientific user visits each year, resulting in more than 1100 refereed publications, the ESRF is recognised as one of the world's most innovative and productive synchrotron light sources. This success is also measured by requests for beamtime from the community of users of the ESRF, consistently exceeding the available beamtime by a large factor. Inspired by the success of the ESRF model, a significant number of ESRF member countries have decided to construct new third generation national SR sources (Soleil in France, Petra III in Germany, Diamond in the U.K. and Alba in Spain).

An essential element for the ESRF's success has been the ambitious refurbishment programme that has allowed science-driven technical innovation to be advanced in crucial areas such as X-ray optics, detectors, sample environment, control systems and accelerator physics. This programme is planned on the basis of a Medium-Term Scientific Programme (MTSP), a scientific road-map covering 5 years which is updated annually, and which provides the scientific justification for the ESRF's Medium Term Financial Estimates.

The longer term upgrade programme discussed here builds on the achievements of the ESRF MTSP with the aim of ensuring to the ESRF a leading scientific position over the next 10 to 20 years. New and refurbished beamlines are proposed to answer new scientific needs, underpinned by a longer term programme to maintain and refurbish the accelerator complex at the heart of the ESRF's activities. Advances in fields such as X-ray optics, detectors and accelerator physics, many of which originated at the ESRF, now allow this ambitious renewal programme covering all aspects of the ESRF's activities. The performance of the beamlines will be enhanced by several orders of magnitude. New scientific areas will be addressed with new highly specialised nano-focus beamlines, with even brighter "hard" X-ray beams, and by renewing beamline components such as detectors, optics, sample environments and sample positioning. Special attention will be paid to the development of advanced imaging techniques and to their combination with X-ray scattering and spectroscopy methodologies.

The technological advances mentioned above, the outcome of more than ten years of research and development in synchrotron science, now permit a qualitative improvement of the ESRF's experimental programme. These improvements require a capital investment that is well above the capital investment budget of the ESRF as given in its present Medium Term Financial Estimate (typically 15 M€). However, it is important to note that the special investment proposed here is considerably lower than what would be required (~1000 M€) to construct a new synchrotron centre with the performance that will be offered by the renewed ESRF. We propose a major capital investment in the ESRF experimental programme, with the aim of keeping the ESRF storage ring and beamlines at the leading edge of research for the next 10 to 20 years and to protect the investment made by the member countries in synchrotron radiation science in Europe, both at the ESRF and elsewhere. In this way, the ESRF will play a major role in the expanding European Research Area.

The principal components of the upgrade and renewal programme are:

- the reconstruction of about one third of the ESRF's beamlines, to have much improved performance with an emphasis on nano-focus capabilities;
- the extension of approximately one third of the Experimental Hall so that beamlines can be extended to about 120 metres and new beamlines built, for nano-focusing applications;
- a prudent programme of improvements to the accelerator complex to maintain the very high brilliance and reliability of the ESRF's X-ray source, and in parallel, the preparation of a longer-term design for a new higher brightness lattice;
- a wide-ranging programme of SR instrumentation development to underpin the beamline and source improvements;
- the development of productive science-driven partnerships including academia and industry.

The intention is that operation costs and staff numbers of the upgraded ESRF will be very similar to present figures. The proposed renewal programme could be started in 2008 and have a duration of five to ten years. Facility "down-time" will be kept as short as possible to minimise disruption of the users' scientific programmes. This upgrade programme for the ESRF has been developed over the last two years and has involved extensive discussion at the ESRF Science Advisory Committee (SAC) and Council, with essential input from the ESRF's scientific user community, directly and via the annual User Meetings. The upgrade programme is thus a response to future scientific needs as expressed by the many scientists from universities and research laboratories who use the ESRF's very intense X-ray beams in their research.

The estimated costs for the different parts of the programme are:

X-ray source upgrades	50 M€
Beamline upgrades and new beamlines (total)	92 M€
Experimental Hall extension	45 M€
Instrumentation development and beamline support	45 M€
Grand Total Capital Investment	**232 M€**

The document is laid out as follows: Section 2 of this report deals with the new and innovative scientific areas to be addressed by the upgraded ESRF and summarises the current situation of synchrotron radiation sources in Europe. Section 3 introduces the renewal programme for the X-ray source, followed in Section 4 by the corresponding plans for the beamlines and scientific infrastructure. Section 5 summarises the preliminary estimates of costs and associated staffing considerations. A summary table of European SR facilities is included as Annex 1 and a report on discussions at the ESRF Users' Meeting in Feruary 2006 as Annex 2. Annex 3 includes preliminary considerations on new and up-graded beamlines.

2. The Scientific Case for the ESRF Upgrade

2.1 Introduction

Synchrotron radiation (SR) sources based on electron storage rings provide intense X-ray beams for a remarkably wide range of scientific studies. Synchrotron light has become an essential tool for investigations in archeology, biology, chemistry, materials, medicine, paleontology, physics and many other scientific disciplines, due to the unique combination of X-ray brilliance, source stability, energy spectrum, polarisation properties and overall reliability of the accelerator complex. Storage ring SR sources such as the ESRF will continue to provide an irreplaceable service to the scientific community requiring analytical tools based on X-rays, even when the X-ray Free-Electron Lasers (XFEL) come into full operation, since XFEL light has very different properties (very different peak brightness and repetition rate and X-ray pulse duration). Consequently, breakthroughs in key areas of science and technology will depend crucially on the continued and improved availability of sources, beamlines and support infrastructures such as that provided today by the ESRF, and over the next 10 to 20 years, by the upgraded ESRF.

The principal motivation of the ESRF's proposed upgrade is to respond to new scientific challenges, and thus to secure in the long term a forefront role for the ESRF in SR based science. The renewal programme described in this paper is designed to maintain ESRF's role as Europe's leading provider of hard X-rays (up to the ~500 keV range) from a very reliable source producing highly stable focused beams (down to ~20 nanometres) with very high intensity. Although the new SR sources being built across Europe will make major scientific contributions, the ESRF's unique combination of extremely brilliant and stable hard X-ray beams, world-leading beamlines and instrumentation and an unparalleled level of scientific and technical support will continue to provide answers to the critical scientific questions of the future.

2.2 Synchrotron Radiation: the European context

This is a period of remarkable change and development for synchrotron radiation science in Europe and across the world. A large number of third-generation SR sources are operating or are under construction, whilst several advanced free-electron laser projects are in the planning or realisation phase. In this section we place the proposed upgrade programme for the ESRF in the context of the rapidly evolving European SR scene.

The Table attached to this paper as Annex 1 lists the beamlines currently operational at SR sources across Europe and summarises their characteristics and areas of application. This information has been derived from the different facility web sites, supplemented by the direct contact where necessary. The Table thus provides an overview of available SR capabilities.

It is important to note that several of the ESRF's Member and Associate countries do not possess national-level SR facilities – the ESRF is their principal SR capability. Consequently, the ESRF's suite of beamlines must complement those available on national sources particularly where harder X-rays are concerned (see discussion below), but must also provide a reasonable coverage of all fields as required by those member nations without their own national facilities.

Several high performance soft X-ray (E = 2 GeV) SR sources have been operating for a number of years. Notable amongst these are ALS, ELETTRA and BESSY, all of which have made very significant scientific advances across a wide range of disciplines. There have been striking advances in angular resolved photoemission with parallel detection which has allowed the study of Fermi surfaces in materials with unprecedented detail and data acquisition rates. The intensity of these soft x-ray sources, coupled with innovative photon and electron optics, has opened the path to new, non-destructive, chemical species and magnetic atom selective microscopies, which in some cases push spatial resolution to the nanometer level. Whilst there is some overlap with activities at the ESRF, notably in areas of research carried out at the ID08 soft X-ray beamline, this work is largely complementary to ESRF studies.

At the other end of the X-ray spectrum, that of hard X-rays (say E > 50 keV), the only European source which can rival the ESRF's performance will be PETRA-III, to be operational from 2009 (at which time the DORIS facility may become unavailable). The small number of beamlines (some 9 have been proposed so far) and the large demand from the German national community will result in only a minor impact on ESRF usage.

The most direct impact on the ESRF can be expected from the new medium-energy sources (SLS, Soleil, Diamond and ALBA). It is however interesting to note that the start-up of the Swiss Light Source has only led to a slight decrease in usage of the ESRF by the Swiss SR community; the return coefficient for scientific use remains close to 1. It is clear that the demand for the ESRF's protein/macromolecular crystallography (PX/MX) beamlines for more routine experiments will decline, especially from the UK biology community as they move to exploit the new Diamond PX/MX beamlines (three are planned for the initial phase of Diamond's operation). However it is reasonable to expect that several years of test and development will be needed before the Diamond (or Soleil, or ALBA) beamlines can rival those at the ESRF in terms of reliability, stability and throughput. With less demand for the more routine projects the ESRF will be able to give more beamtime to the more advanced biological projects such as protein complexes and membrane proteins that often require screening thousands of crystals. This procedure has been greatly facilitated by the automation of the ESRF's MX beamlines equipped with large detectors.

While Diamond and similar synchrotrons will have very high brilliance for X-ray energies up to at least 20 keV, a consideration of all factors governing the experimental signal strength (beamline divergences, apertures, etc) leads to the conclusion that the cross-over energy where ESRF beamlines become superior is relatively low, and is calculated to lie below 10 keV.

Where the various free-electron laser projects are concerned, the impact on the ESRF is expected to be even less direct. The very low energy sources already operating (e.g. FELIX operates in the infra-red and far-infra-red) provide experimental facilities for atomic and molecular spectroscopies and have strong programmes in biological fields (e.g. bio-medicine) in energy regimes far from those of the ESRF. The field of linear accelerator based FEL facilities is evolving rapidly thanks to demonstrations of the SASE concept in the visible and VUV region. This progress is exemplified by the successful operation of the VUV FEL (FLASH) at DESY which is opening up new and exciting fields of science on ultra-short time scales. The ambitious soft X-ray and X-ray projects such as FERMI at ELETTRA and the European X-FEL at DESY are several years away from routine operation. Similar projects in the US and Japan are at a comparable state of advancement. Whilst these projects will make new time domains accessible, initially their major customer base will lie principally with the high power laser and atomic-and-molecular scientific communities. In addition, the number of beamlines planned is relatively modest. There will also be a significant period of test and development before the X-ray FELs will become routine user facilities with reliable and well understood operation modes as at the ESRF and the other third generation SR sources.

2.3 New and expanding scientific fields

Synchrotron Radiation science owes its success to its impact in the science of materials considered in the widest sense. The ESRF offers first class facilities for a wide range of scientific programmes and aims to maintain and improve its engagement in these areas. This will continue to enable existing scientific communities to tackle both fundamental and applied problems. The much improved scientific capabilities of the ESRF on completion of the upgrade programme will be exploited in five broad scientific areas: **nano-science and nano-technology, pump-probe experiments and time-resolved diffraction, science at extreme conditions, structural and functional biology, soft matter and X-Ray imaging.** Below we discuss each of these in turn and provide illustrative examples of the types of new science made possible by the ESRF upgrade.

2.3.1 Nano-science and nano-technology

The ESRF is an essential tool for structural and dynamic investigation of materials from macroscopic (millimetre) dimensions all the way down to the truly molecular (Ångstrom to nanometre) level. Many new areas of study in biology, chemistry, environmental sciences, materials science, medicine and physics have been developed, notably by the provision of brilliant and stable micrometre sized X-ray beams. Based on recent ESRF advances, the optimisation of all X-ray beamline components and beam optics will allow X-ray beams down to around 20 nanometres, enabling research in new scientific areas such as innovative “designed” nano-materials, the fertile interdisciplinary area of soft matter/biological materials, and nano-scale electronic/spintronic components.

Innovative materials in general, whether of biological origin or man-made, have properties which almost always depend on the specific hierarchy of chemical components, organised at different length-scales. Therefore, an understanding of macroscopic function requires an understanding of microscopic structure and dynamics on all length-scales down to the molecular and atomic level. This is particularly important for structural investigations on composites, polymers, ceramics, geo-materials, structural/functional materials, smart materials and biomedical materials. These investigations must address *in-situ* studies of specific behaviour, such as phase transformations, dynamics, reactions, simulated manufacturing conditions, deformation and damage, and environmental consequences.

Fundamental and applied materials research is a crucial area of high growth, underpinning the technological developments and competitive advantages of the 21st century. In this respect, the present lack of analytical tools and limits in technology explain our poor understanding in bridging the gap from macroscopic function to its atomic/molecular origin. This explains why, for example, we are still very far from assembling complex biological materials such as bones and wood.

Nano-technology is starting to provide the tools for the bottom-up assembly of complex materials. This technology is expected to replace eventually the top-down strategy used until now by the electronics industry for the assembly of complex electronic components and, for example, will provide higher storage-density chips. The progress of these developments implies the need for new nano-analytical tools to be made available besides those already existing at longer length-scales. Traditional length-scale sensitive techniques are based on local area electron probes or other scanning probe techniques, which are not bulk-sensitive. The availability of synchrotron radiation micro- and nano-probes now make unique *in situ* capabilities possible. SR based analytical techniques (diffraction, imaging and spectro-microscopies) will play an important role by offering 3D information that is both time-resolved and chemically selective.

The ten years of experience at the ESRF in developing instruments with micron or sub-micron lateral resolution shall be used as the foundation for upcoming new nano-science projects. Several crucial issues can be identified for a successful development of these programmes:

- **Beamlines**: SR probes aiming for the smallest possible spot size (e.g. 3D-tomographic, 3D-diffraction imaging, 2D-mapping and grazing-incidence techniques) will require very long and stable beamlines, possibly with intermediate virtual sources. Improvement of the synchrotron source performance (e.g. stability, photon flux and emittance) will be of primary importance in such programmes. These instruments, moreover, will need to retain the capacity to address efficiently materials studies at longer (micron and millimetre) length-scales to provide the full picture. This implies, for example, the availability of high energy X-ray diffraction and imaging beamlines with multiple stations, each one adapted to the relevant length-scale.
- **Optical systems**: The ESRF has built and sustains a strong research and development programme in focusing optics, including very fruitful collaboration networks with external academic partners. Compound refractive lenses, Fresnel zone-plates, multilayers and mirrors are used routinely at the ESRF. The ESRF is well placed, therefore, to take a leading role in coordinating the further development of focusing optics and in making them available to the upcoming micro- and nano-focusing beamlines at the ESRF and at national SR sources.
- **Sample environments**: Handling samples of nanometre dimensions will require the development of new and challenging tools, as well as highly adapted sample environments which will range from very exotic extreme conditions (see 2.3.3) to “harsh” environments appropriate to the specific problem under investigation.
- **Nano-Science Centre**: The creation of such a centre at the ESRF with the necessary laboratory space and infrastructure will create opportunities for research and development in optics, sample environment and analytical techniques. The centre will be organised in terms of a partnership with outside laboratories, specialised in nano-technologies and nano-analytical tools. A coordinated access to various instruments (including beamlines and laboratory instruments) providing to the community complementary nano-analytical tools

(spectroscopy, diffraction, and imaging) would constitute a unique platform worldwide.

The first steps to develop suitable nano-science instrumentation have already been initiated by the ESRF through the pilot upgrade projects of ID11, ID13 (nano-diffraction) and ID22 (nano-tomography). In the longer term, these and other new beamlines should merge into the nano-science centre. This will be an integrated structure, which will comprise suitable satellite laboratories providing the infrastructure necessary to carry out SR-based analysis and to promote the optimal use of the dedicated beamlines. This centre will then have the firm basis necessary to develop effective and productive science-driven collaborations around specific scientific projects.

New Science: illustrative examples

Future nanofocus beamlines will strive for the smallest possible focal spots, which have been predicted to be around 20 nm. This will provide exciting opportunities for studying *functional biological units* by imaging techniques. Thus a major focus of tomographic techniques, such as fluorescence tomography, will be on cell biology. Following in situ the pathways of trace elements and metal ions into intact cells and subcellular components with nanometre resolution will present a major technical advance as compared to ex situ electron or ion-probe techniques. Tomography techniques will also address the chromosome distribution in cell nuclei and the search for nuclear territories, which are thought to be linked to RNA transcription.

The "competition" of imaging with diffraction techniques will be very fruitful. Thus focal spot sizes of about 100 nm will allow both small-angle and wide-angle scattering studies, which combine *local probing* with structural resolution on length scales down to *atomic resolution*. These features are required to study the adaptation of hierarchical biocomposite structures (e.g. wood or bones) to external stimuli such as tensile stress. It should not be overlooked that very long beamlines will provide the possibility of optimising focal spot size and beam divergence. The development of flexible X-ray optical systems, such as compound refractive lenses, will have a major impact on single crystal diffraction where one might screen across a crystal for the best diffracting section or wish to bathe a larger crystal in X-rays.

2.3.2 Pump-probe experiments and time-resolved diffraction

The study of processes and reactions that occur at time scales from nanoseconds to hundreds of seconds is being actively pursued at several ESRF beamlines using spectroscopic, scattering and diffraction methods. These studies are highly demanding in terms of sample environment and will continue to be the driving force behind much of the detector development at the ESRF. In addition the ESRF has pioneered time-resolved diffraction studies on biological systems and chemical bonding with a beamline partly dedicated to this important scientific field. These world-leading investigations exploit the time structure (down to ~100 picoseconds) of special storage ring operation modes. These studies will explode in importance when the new XFELs become available, as demonstrated by the ground breaking work at the TTF2 facility at DESY, in the VUV, and in the X-ray region at the SPPS at SLAC. Instrument optimisation and new beamlines at the ESRF will permit both diffraction and spectroscopic investigations, setting the scene for sub-picosecond XFEL science in the decades after 2010.

Picosecond time-resolved diffraction has proved to be a very powerful tool to track the structure of molecules as they change shape and composition during a chemical reaction. These experiments are performed in a pump and probe fashion: femtosecond laser pulses excite a sub-set of molecules in the sample, and delayed X-ray pulses probe the structure at a given delay. The diffraction patterns are recorded on a CCD detector and by varying the time delay, from 100 picoseconds to milliseconds, a real-space film can be made by Fourier inverting the diffraction patterns. Laue diffraction studies are usually conducted in the 4-bunch mode of storage ring operation, which gives the highest number of photons in a single shot. The best example is the recording of the dissociation of CO from the myoglobin complex MbCO. One of the key questions to address in the next few years is the role of water molecules in protein dynamics. Indeed, new experiments have been able to resolve water motions in certain proteins.

Solution Phase X-ray Diffraction (SPXD) is another field where the ESRF has made important contributions. These experiments use a moving sample, which makes it possible to study irreversible reactions at high frequency, ~1000 Hz. Using the intense pink beam from a single harmonic of a short period in-vacuum undulator it is now possible to acquire diffraction spectra, with 100 ps time resolution, at a rate of 20 per hour. The spectra measure the laser-induced change in atom-atom correlations during a chemical reaction. The experiments have shown the signatures of the formation and breakage of bonds, geminated and non-geminated recombination of products, the solvent structure around the products and the hydrodynamics of the solvent medium (i.e. the change in temperature, pressure and density). These experiments are analysed using molecular dynamics simulations (MD), classical hydrodynamics and statistical theory of liquids.

Interest is turning towards larger and more complex molecules. The recent results obtained for the allosteric transition of haemoglobin show that studies can be extended to macromolecular assemblies. There are strong indications that protein dynamics (folding/unfolding) can be studied in the natural environment in this way. Nano-scale crystals should also be mentioned, where plasmons can be excited by laser pulses. The electron energy is transported, via the electron-phonon interaction to the lattice, and coherent vibrations have been observed in powder diffraction. Very small nano-particles with diameters down to 5 nm are also likely to be paarticularly interesting as an intermediate between a molecule and a crystal (giving rise to Debye scattering rather than crystal diffraction). The physics of such many-body molecules will undoubtedly become a fascinating area of research.
An increased effort must be made to further develop time-resolved sub-nanosecond X-ray scattering and spectroscopy through beamline development and by exploiting new storage ring operating modes to provide new possibilities for these techniques.

New Science: illustrative examples

A future beamline dedicated to pump and probe experiments will be able to record chemical reactions at true atomic resolution using hard X-rays (30-40 keV). By extending the Q range from 0.1-10$Å^{-1}$ (as currently available on ID09B) to *0.1-20* $Å^{-1}$, it will become possible to *track atomic positions* in chemical reactions down to a time resolution of *50 picoseconds*. In state-of-the-art experiments on ID09B we can only see the change in population between quasi-stationary states in chemical reactions. The new beamline will, for example, be able to resolve the cooling of vibrationally excited nascent molecules.

The photosynthetic splitting of water into molecular oxygen and hydrogen is a fundamental biocatalytic reaction that provides the oxygen we breathe. The different catalytic reaction steps in the oxygen evolving complex (OEC) of plants are still not fully understood. In order to elucidate the reaction kinetics and intermediates in the final steps where O_2 is released, time-resolved X-ray absorption and emission spectroscopy of manganese in the OEC with nanosecond resolution will give valuable insight into the electronic and structural changes. Furthermore, natural photosynthesis is mimicked in dye-sensitized solar cells. Here the time resolution has to be pushed into the picosecond and even sub-picosecond range in order to track the fast electron transfer between the dye (e.g. ruthenium polypyridyl complexes) and a large bandgap semiconductor (e.g. TiO_2). The element-specific probe of the electronic structure and local coordination provided by inner-shell spectroscopy will permit investigations of problems that presently cannot be studied by any other technique.

2.3.3 Science at extreme conditions

In parallel to the increased performance of the X-ray source and the beamlines, the further development of more complex sample environments is a key issue. Experiments at extreme conditions of temperature (milli-Kelvin to 5000 Kelvin), pressure (up to 5 Mbar) and magnetic field (up to 50 Tesla, constant and pulsed) are already feasible, or within reach. The combination of the various synchrotron radiation-based techniques (diffraction, small-angle scattering, absorption spectroscopy, inelastic scattering and nuclear scattering) will provide valuable information on the structure, dynamics, electronic and magnetic properties under previously unexplored thermodynamic conditions, relevant in a large range of fundamental and applied science disciplines, from biology to cosmology.

The synthesis and *in situ* characterisation of new materials under these conditions will provide crucial information for industrial applications and on the performance of materials, essential input to the most advanced energy programmes such as ITER and NIF. Knowledge of the structural and elastic properties of elements, compounds and minerals relevant for earth and planetary science will provide new insights into the evolution and composition of the planets of our solar system. Magnetic spectroscopy of molecular magnets at milli-Kelvin temperatures will contribute to the basic research effort towards the development of a future quantum computer. Studies in magnetic fields of unprecedented strength will lead to the discovery of novel effects and will have a decisive influence on the better understanding of semiconductors, superconductors and magnetic materials. The use of hard X-rays as a probe of materials subjected to intense magnetic fields will offer unique possibilities, as is the case for infrared spectroscopy, where the (soft radiation) free electron laser ELBE at the high magnetic field laboratory in Dresden will allow experiments up to 100T.

Although an increasing number of different experimental methods have been employed over the last decade, X-ray diffraction is expected to remain the most widely used technique in the context of extreme conditions research because it provides fundamental structural information that is the basis for other synchrotron techniques. This area requires a major effort in the development of new beamlines, new instrumentation (particularly in sample environment and X-ray detectors), and in the related scientific infrastructure.

New Science: illustrative examples

The construction and installation of a multi-analyser spectrometer capable of retrieving the sample's complete phonon dispersion curve *at only one setting* of the spectrometer (and sample) would enable, for example, the study of single crystal minerals under pressure and temperature conditions of the Earth's mantle which can only be reached by *combining diamond anvil cell techniques and laser heating*. This is currently impossible due to low count-rates and the difficulties of orienting the sample crystal (in its complicated sample environment) at many different angles.

Quantum effects in magnetic systems are enhanced by low dimensionality, low spin and frustrated interactions. Two-dimensional “spin dimer” systems, where the magnetic interactions are strongly anisotropic and the spin dimers form spin singlet ground states, are especially interesting. By applying an external magnetic field *above 20 Tesla*, we may close the spin gap and form a gas of spin triplets. At certain characteristic field strengths plateaus are observed in the magnetisation curves. These arise from the crystallisation of the triplets into superlattices. Their precise nature is still controversial as no direct microscopic probes are currently available. Through studies of the corresponding superlattice reflections under extremely high applied magnetic fields (above 20T), X-ray *resonant magnetic* scattering will provide direct insight into the long range interactions of the triplets. In addition, X-ray spectroscopy, in particular *resonant inelastic* x-ray scattering, will complement these data with information on the relevant energy scales and local symmetries.

2.3.4 Structural and functional biology and soft matter

The use of synchrotron light for diffraction experiments has been essential for the exponential growth of knowledge of the three-dimensional structures of biological macromolecules. The field of structural biology has been revolutionised by access to synchrotron radiation. Experiments that were previously difficult have become routine and the “impossible” ones are now achievable. The success of the macromolecular crystallography beamlines at the ESRF is reflected in the fact that all of the new European synchrotron sources will have beamlines for macromolecular crystallography, giving extra capacity for experiments in structural biology. This provides an ideal ground to push further for innovation and challenges the ESRF to develop new capabilities to address the most advanced biological problems.

The current revolution in biology will continue to require extremely detailed structural information on increasingly “difficult” samples, such as membrane proteins and macromolecular assemblies. New highly automated nano-focus beamlines with high-throughput capabilities will be necessary for the screening and measurement of crystals made out of these challenging assemblies. These crystals will have increasingly large unit cells and decreasing sample size. The new beamlines will therefore need to be complemented by both new detectors and new sample positioning systems. These are the mandatory conditions to increase throughput and allow data acquisition strategies to minimise problems associated with radiation damage and crystal quality. An overall gain of at least a factor of 100 can be foreseen compared to the present situation. This improvement will have a great impact on the European initiatives to combat diseases and other health related problems in which structural information is the key factor. The study of proteins related to human health is not trivial and will often require analysis of numerous crystals before a suitable one is found. The handling of these problematic samples can be optimised through a further development of the automation process at the ESRF MX beamlines. This constitutes the motivation for the ESRF to start the development of a Massively Automated Sample Screening Integrated Facility (MASSIF), to carry out the efficient screening of crystals in order to obtain the best possible crystallographic data. With MASSIF it should become routine to screen, analyse and rank hundreds of samples before data collection is initiated.

Crystallisation represents one of the bottlenecks in the protein structure determination and about 20 to 40 % of the proteins present such severe difficulties in crystallisation that they are not accessible to diffraction techniques. The application of SAXS/WAXS experiments for soft condensed matter research is well established, but its potential has not yet been fully exploited in the study of biological samples. Valuable information that can be used to guide the protein crystallisation experiments can be obtained from screening protein solutions under many different conditions. A detailed structural interpretation of the low resolution structural data from SAXS/WAXS experiments can be obtained using the tools of bioinformatics in combination with the wealth of information from known protein structures.

An understanding of the relation between structure and function in biological systems requires structural information for the system under many different experimental conditions, necessitating ancillary instrumentation associated with the beamlines. The macromolecular systems that are targets for investigations are becoming increasingly complex and with this increase in complexity it is likely that the samples will not generate large well ordered crystals or possess sufficient symmetry to make cryo-EM techniques feasible. By the use of coherent diffraction it is possible in principle to reconstruct structural information at spatial resolutions comparable to the best electron microscopy (10 Å). X-rays are more suited to examine samples thicker than 50 nm due to their greater penetration depth. One of the MX beamlines will be developed for coherent diffraction with the aim to provide structural information on whole cells, sub-cellular cultures and viruses. The information on whole cell behaviour is also important for the development of the biomedical research at the ESRF. Single cell studies provide an important basis for the continued development of synchrotron radiation therapy of brain tumours towards appropriate clinical protocols.

The integration of information on biological systems obtained from different experimental synchrotron based techniques is essential for the scientific developments in the emerging field of system biology. This combination of different experimental techniques has been critical for the development of soft condensed matter research; an even stronger cross-fertilisation between structural biology and soft matter in the future can be envisaged. Both soft matter and biomaterials research are undergoing rapid change, with a major impact on future technologies (energy storage devices, self generating materials…). A precise knowledge of the structure and physical properties with atomic resolution is of primary importance for the development of nano-bio-science as a research field of rich potential. In this area new beamlines dedicated to very small samples will enable an expansion of soft matter research at the border between macromolecular crystallography and traditional soft matter science.

New Science: illustrative examples

A full understanding of the unique relations between structure and properties of soft matter and of biological processes in terms of the chemical and physical behaviour of the large and small molecules in a cell requires information on the relation between structure and function at *many different length scales*. These range from the detailed picture of atomic positions that can be obtained by diffraction from single crystals to images displaying the internal structure of an individual cell.

The large scale structures of cellular life and cellular machinery are generally studied by transmission electron microscopy (TEM). In this method thin slices (~0.5 µm) of the cells are required due to the limited penetration depth of the electrons. Though TEM has been successful in determining highly symmetric virus structures, it is not applicable to complete cells. X-ray *coherent diffraction imaging* has recently demonstrated the dual advantages of increased penetration depth which will enable the imaging of intact cellular systems and the capacity to reconstruct non-periodic objects. A beamline at ESRF capable of achieving nanometre resolution images of biological samples by coherent diffraction imaging will open new and unique scientific opportunities for the biological sciences.

2.3.5 X-Ray imaging

X-ray imaging with its many variants (including microscopy in fluorescence-, spectroscopy- and diffraction-mode, three-dimensional imaging using tomography methods, and the exploitation of coherence) is revolutionising the perceptions in the scientific community of the possibilities offered by SR in general and by the ESRF in particular. X-rays bring many specific advantages to imaging: the techniques are typically non-destructive and can be selective to a wide range of properties (density, chemical element, chemical bond, spin, magnetic moment, strain, surface versus bulk, order versus disorder) with extremely high sensitivity.

It is clear that these imaging methods will increasingly develop over the next years, both from a technical point of view and in terms of the domains of application. X-ray imaging techniques are being applied today in an increasing number of fields. They are not only applied to physical, materials science and engineering topics, but also to new areas of interest that include medicine, environmental sciences, engineering, archaeology, palaeontology, and human heritage sciences. Importantly, the evolution of these techniques towards high spatial and temporal resolution, *in situ* experiments (in particular for microanalysis at extreme conditions) and precise quantitative measurements is permitting a host of new research subjects. Examples include materials science, where the dimension of the structures under investigation range from 100 mm down to 10 nm, nano-technology where the important structures are of 50 nm size and below, as well as bio-materials and soft condensed matter (soils, micro-structure, composition, plasticity of a wide range of materials …).

The ESRF has always been at the forefront of X-ray imaging, exploiting the various advantages described above to the profit of the scientific community. ESRF beamlines allow the combination of the photon energies and beam coherence needed for three-dimensional analysis with appropriate advanced sample environments (including extreme conditions) and very high spatial and temporal resolution. This combination is not readily available at other SR facilities and the ESRF should pursue the development of these techniques, taking full advantage of the specificities of the X-ray source. This implies pushing the spatial resolution, presently in the 100 nm to 1 µm range, to gain one order of magnitude (to achieve the 20 nm scale), thereby facilitating nano-science research. Temporal resolution must be improved (to the millisecond range) to investigate evolving processes (fracture propagation, phase transformations …). Imaging of biological samples poses special problems, in particular that of sensitivity to radiation. The “dose problem” can be substantially relieved through investment in detectors providing simultaneously high resolution and efficiency. Demand for imaging techniques is increasing very rapidly and upgrades to detectors, optics, sample positioning and data acquisition are required to cope with this demand.

New Science: illustrative examples

A long "nanoprobe" beamline will allow routine experiments that are not feasible today. An outstanding example is the chemical imaging of biological cells. To achieve this implies being able to scan the cell with a spot *small with respect to the cell dimensions* and intense enough to collect the fluorescence.

A preliminary experiment has been performed at beamline ID19. Some of the features required for a long nanoprobe beamline exist at this beamline, but not, for instance, the extreme level of stability required. The image obtained in this "tour de force" experiment shows the location and content of Pt in a cancerous cell with a *resolution of 0.3 µm*. Indeed the detection, localisation, quantification and determination of the chemical state of (metal) trace elements in cells is of crucial importance for a broad range of biomedical topics, which include brain diseases associated metabolism disorders, nano-bio-technologies and bacterial metabolism under extreme conditions. The recent results obtained at 3rd generation hard X-ray sources demonstrate unequivocally the scientific potential of an optimised long nanoprobe beamline for biomedical topics, as well as for applications in materials science.

3. X-Ray Source Upgrades

3.1 Introduction

The performance of the ESRF's X-ray source can be further enhanced by increasing the electron current and by operating in a "top-up" mode. In parallel, work will continue on the design of a new magnetic lattice, to be accommodated in the existing tunnel but with a significantly reduced horizontal emittance. These investigations are aimed at providing X-ray beams of even higher brilliance and intensity to permit new science at the ESRF's beamlines. A very important boundary condition for these developments has been emphasised continuously by the User community: *improvements of the brilliance must not decrease the performance of the storage ring in terms of reliability and stability.* Beam stability is therefore an essential parameter for the possible upgrades of the storage ring. Instabilities can arise from long term drifts and high frequency motions. In this respect, the operation of the machine in a top-up mode can constitute a clear benefit.

3.2 Top-up injection, new timing modes and current Increase

Topping-up is an attractive option for ensuring extreme beam position stability as well as stable heatload on beamline optics. A top-up mode will be developed for all filling modes. Its routine use in multibunch filling modes will need a futher study taking into account safety issues, beam stability during refill and running costs.

The use of topping-up in 16 and 4 bunch modes appears attractive in view of the short lifetime of these modes and the option for smaller vertical emittance. A top-up in the hybrid mode, together with the implementation of a fast chopper on the time-resolved beamlines, would permit time-resolved diffraction and spectroscopy studies to be run simultaneously with all other beamlines which require the full current. With the new High Quality Power Supply (HQPS) system about to be ordered, as well as a few modifications to the injector system, this could become a standard mode of operation within three to five years. New filling patterns will be studied to better accommodate the needs of the Users. In particular, it appears crucial to satisfy the majority of the ESRF Users with a long lifetime multibunch mode, as uniformly filled as possible, while providing simultaneously a useful beam for the science involving time resolved experiments (for example ID09, ID18, ID22...).

It is also planned to increase the ring current to 300 mA in User Service Mode (USM). This will await the installation of the new crotch absorbers and appears possible within a reasonable time frame (three to four years). The new crotch absorbers currently under manufacture will have a higher thickness of "glidcop" alloy to reduce the corrosion responsible for the failure of the Cell 15 crotch absorber in March 2005. While high frequency multibunch instabilities presently limit the current to 200 mA, stable operation up to 300 mA is considered to be feasible in the uniform filling mode thanks to the digital bunch-by-bunch feedback system presently under development. A further increase to a current of 500 mA is envisaged in the longer term but will require more refurbishment. A number of vacuum chambers of the ring need to be redesigned and changed. In addition, new radio frequency cavities with heavy damping of higher-order modes need to be developed and tested in order to replace the present cavities. The time horizon for a 500 mA ring current is estimated to be between five and ten years.

3.3 New undulators and canting options

To increase the number of independent instruments on a beamline, it is desirable to split the straight section to enable two shorter insertion devices (IDs) generating the radiation at different angles to be installed, resulting in a "canted undulator" geometry. Such a set-up, with a 1.5 mrad angle between the two undulators, has been implemented successfully on two beamlines for macromolecular crystallography using the ID23 section. For future developments, a larger angle is desirable to further decouple the instruments on each branch and to make optimum use of the limited floor space in the Experimental Hall. A preliminary study has shown that an angle of about 6 mrad should be possible; detailed study is needed to confirm this. The beamline front-end will need a completely new design as well as that of the dipole vessel and the crotch absorber vessel. Chicane magnets generating the 6 mrad angle deflection as well as new sets of 2.2 m long undulators, preferably in-vacuum or of the "revolver" type, will be implemented. Machine studies will be conducted to investigate if the length of the ID straight section could be increased by removing the last quadrupole on each side of the straight section (leading to a gain of 1 m) and possibly some sextupoles on a few straights (which would free another meter). A decision on such lattice changes could be made within a year. While no net increase in the number of beamlines is currently envisaged, carrying out the modifications described above (to the dipole vessels, crotch absorber vessels and front-ends) for a limited number of beamlines would introduce the flexibility needed so that the ESRF can respond, in the future, to developments in scientific priorities.

3.4 Very short (ps) pulsed X-ray beams

There is a large interest in the new scientific opportunities provided by short (ps) X-ray pulses. Since the pulse is naturally long in storage rings (several tens of ps), exploring the possibility of producing short pulses (in the ps range) while keeping a high flux requires the development of innovative techniques such as the slicing of the beam by means of deflecting RF cavities ("crab" cavities). The feasibility issues (lattice, cavity design, operational impact on users …) need to be studied and quantified before considering the implementation of such a scheme. Simulation and theoretical work on this possibility will be carried out. If successful, RF cavity design, could start within one or two years. In view of the long lead time needed for cavity prototyping and production, a delay of five to six years for user implementation appears as the minimum required.

3.5 Lattice studies

The lattice of the ESRF storage ring is of the Double Bend Achromat type (two bending magnets between successive ID straight sections) with residual dispersion in the ID straight section providing an effective horizontal emittance of 4 nmrad. Two scenarios of lattice upgrade have been envisaged. To be cost effective, the constraint of keeping the tunnel, shielding and beamlines untouched was imposed, while replacing all magnets, associated power supplies and vacuum chambers. One scenario consists of implementing a Triple Bend Achromat lattice. The second approach consists of implementing a Double Bend Achromat lattice similar to that presently in use but with special bending magnets providing a variable magnetic field along the beam path. Both approaches aim at an effective horizontal emittance around 1 nmrad (compared with the current value of 4 nmrad). Even smaller emittances can be achieved for "model" storage rings of significantly larger circumference than that of the ESRF's Machine. Consequently, in parallel with the calculations described above, the staff of the Machine Division have revived their previous work on the design concept of the “ultimate storage ring”, as advised by the ESRF SAC.

A number of challenging issues are raised by the attempt to improve substantially the emittance within the constraints listed above. On the technical side, the main difficulty concerns the design of magnets of unprecedentedly small apertures, possibly combining quadrupolar and sextupolar functionalities in a single magnet. This innovative design will require prototyping. However the major concern deals with the non-linear beam dynamics behaviour in these small emittance lattices. The correction of the aberrations induced by the increased focusing implies the use of much stronger sextupoles that limit the dynamic aperture to very low values, and this is the main challenge to the feasibility of these lattices. Studies are still ongoing to improve our understanding of these issues. The research and development programme to design a new high-performance small-emittance lattice constitutes an interesting and important challenge for the ESRF Accelerator Group and is thus indispensable to retain a high level of motivation.

3.6 Summary of source upgrades

The upgrade of the ESRF storage ring is envisaged as a continuous development project, comprising improvements to be realised during the proposed five year ESRF renewal programme, along with longer term studies to establish the feasibility and the opportunity to completely change the existing storage ring with a new accelerator complex. The immediate upgrade will develop, on the existing machine, increased stored current, the top-up possibility to improve the performances of special operation modes and front-ends adapted for canted insertion devices.

X-ray Source Upgrades - estimated cost: 50 M€

4. Beamlines, Experimental, Scientific and Computer Infrastructure and Instrumentation Developments

4.1 Introduction: optics and nano-focusing

New science is the driving force behind the ESRF's long-term strategy. A common feature of the new science summarised in Section 2.3 is the need for ever-smaller beams of extremely high brilliance This trend towards nano-sized beams constitutes the logical evolution of a trend which has been evident from the early days of ESRF operation. In the ESRF Foundation Phase Report (Red Book) it was expected that a "micro-focusing beamline" could deliver a beam size of ~30 µm and that most beamlines would operate with a beam of about 1 mm dimension. Today, the limiting capability of the "micro-focusing" beamlines is to deliver X-ray beams of less than 100 nanometre, but this performance remains far from routine. A "standard" beamline operates routinely with sub-millimetre beams. The pressure from scientists and users to have routine beams of 10 µm or less (down to 1 µm) is enormous. The reasons for this are multiple and reflect many facets of the scientific case outlined in Section 2. For example they are needed:

- to study small crystals of all materials, protein crystals, novel materials, nano-structures, quantum confined structures;
- to investigate efficiently samples in extreme and exotic thermodynamic conditions; pressures up to 3 Mbar; temperatures up to 5000 K and down to the sub-Kelvin region; magnetic fields up to 50 Tesla; combinations of such conditions;
- to develop advanced techniques, such as coherent X-ray scattering and spectroscopy and, more generally, to combine imaging techniques with X-ray scattering and absorption techniques to develop new X-ray methodologies.

Recent work performed by teams of ESRF scientists and external collaborators has demonstrated a world leading performance in focussing X-ray beams of about 20 keV to less than 50 nm, using either a dynamically bent graded multilayer device or an assembly of compound refractive lenses. In order to implement efficient focusing options in the sub-micron region on generic beamlines providing stability and compatibility with sophisticated sample environment equipment, it is necessary to construct optical devices capable of very large source demagnification, in the range 1 in 1000 to 1 in 10,000. These requirements pose a number of new challenges. Not only the optical quality of reflecting and refracting devices must be outstanding, but also the temperature and vibration stability of the experimental environment must satisfy extremely demanding criteria.

The "long" beamlines to enable these demagnification ratios need to be sensibly longer than a typical ESRF beamline, which is ~ 50 m, extendable to a maximum length of 70 m. In fact, with a 1:1000 demagnification at 50 m from the source, only 50 mm would be available between the centre of the optical device to the focal spot. This could be increased to a much more comfortable value of 120 mm if the beamline length could be extended to 120 m. The possibility to have a secondary source can be a key parameter for the improvement of the stability and the overall control of the critical parts of an experiment using very small beams. This option, if implemented efficiently, also requires a beamline at least twice as long as that typically possible today. Already, as part of the ESRF's Medium Term Scientific Plan, two pilot nano-diffraction beamlines (ID11 and ID13) are being extended to achieve focal spots in the nanometre range. We propose to create the conditions for the construction and exploitation of a number of long beamlines, up to a maximum length of 120 m, at the ESRF.

This section is organised as follows: in Section 4.2 the extension to the Experimental Hall needed to house long beamlines is discussed. Section 4.3 lists the new and modified beamlines envisaged. Section 4.4 is dedicated to the development of the new instrumentation necessary to exploit the new beamlines, while Section 4.5 deals with computing needs and Section 4.6 comments on possible future scientific partnerships.

4.2 Extension to the Experimental Hall

As one of the core elements of this strategy we propose the enlargement of approximately one third of the existing Experimental Hall. It is planned that about ten beamlines can be accommodated of the length needed for nano-focus applications. An attractive feature of this extension is that in doubling the length of an undulator beamline, one also doubles the space available at the sides of the beamline. Therefore, the floor space will be compatible with two undulator beamlines in the Experimental Hall emerging from the same straight section. Stimulated by this very interesting option, as discussed above in Section 3.3, the ESRF Machine Division proposes to develop further the concept of mounting two canted undulators in the same straight section. With a maximum total canting angle of 6 mrad and a new front-end, it will then be possible to install two completely independent long undulator beamlines in the same straight section. This will cost a factor of approximately two in intensity, partly recovered by the planned current increase.

This possibility is particularly attractive because the extension of about one third of the Experimental Hall would allow the reconstruction of more than 10 of the ESRF beamlines, with increased length, and at a later stage even a larger number with the installation of canted undulators where such an option is justified by the scientific case for the beamline. The present upgrade plan is based on preserving a portfolio of around 30 public beamlines of the highest quality at the ESRF.

In summary, the extension of one third of the ESRF Experimental Hall, coupled with the development of high-angle undulator canting provides an innovative and economically attractive way to install long beamlines (potentially up to a length of ~120 metres) for nano-focus applications, with the potential to increase the number of insertion device beams available for science, thereby enhancing and preserving the very large capital investments made in the ESRF.

Building beamlines of length approximately 120 m will require a partial 20 m radial extension of the Experimental Hall. A preliminary feasibility study has been carried out, taking full consideration of the following constraints:

- possibility of 120 m long beamlines on ten front-ends;
- maintaining the height of the existing overhead crane;
- maintaining the continuity of the freeway between the Experimental Hall and the extensions;

- facilitate the possibility of rebuilding two to three times the surface area lost (offices and laboratories) to the extensions
- possibility of additional beamlines with canted undulators.

Given the geometry of the ESRF site, three extensions are possible as shown in Figure 1, from either side of the footbridge between the central building and the Experimental Hall, and south of the Experimental Hall (on the Vercors car park). These three extensions will call for a reappraisal of the roads and networks around and inside the Experimental Hall as well as significant modifications to the parking areas. The extensions foreseen conserve the possibility of building two extra-long beamlines, over 150 m, on ID16 and ID18.

The three extensions proposed could accommodate at least ten long beamlines and, in terms of useful surface, represent:

- Extension of the Experimental Hall: 8000 m²;
- New laboratories and offices on the periphery of the three extensions: 9700 m²;
- Three satellite buildings of a total surface of 4500 m².

This leads overall to a potential new useful surface area of about 22000m² (30% of that existing at ESRF). Figure 2 presents an artist’s impression of the extension of the Experimental Hall and one of the new satellite office/laboratory buildings.

Experimental Hall extension - estimated cost: 45 M€

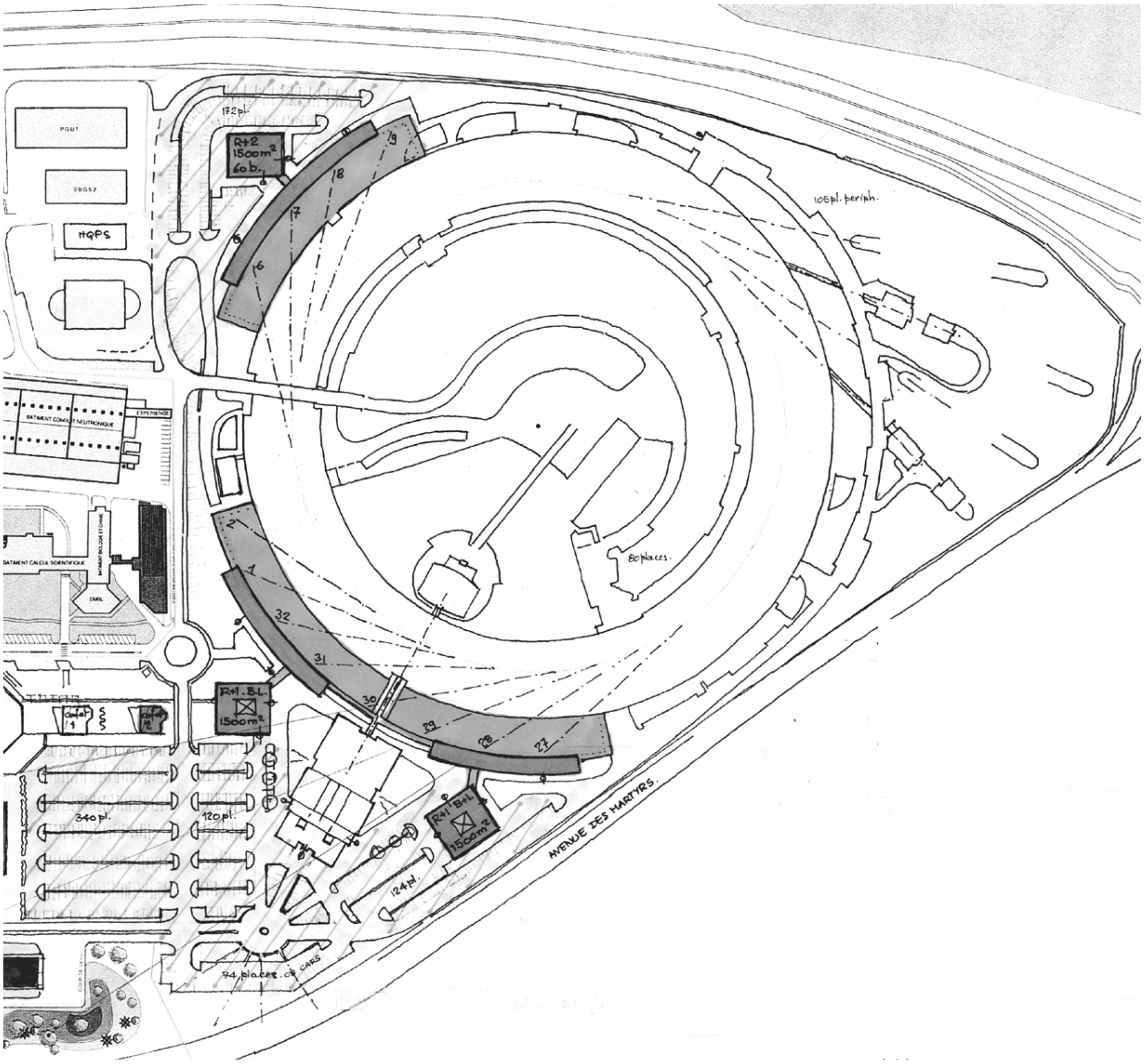

Figure 1: ESRF Experimental Hall extension

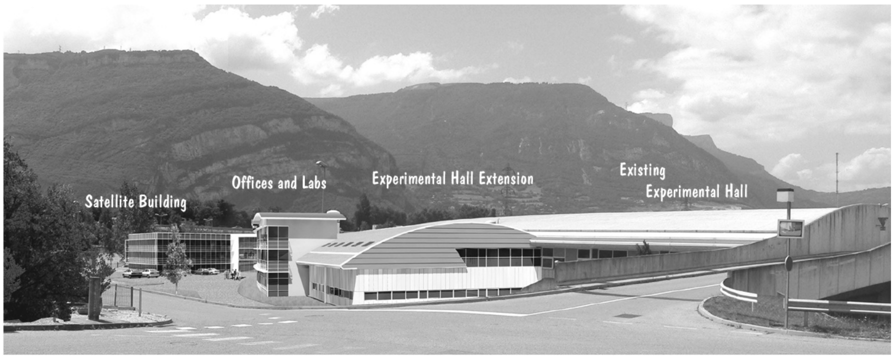

Figure 2: Artist's impression of the extended Experimental Hall and a satellite building

4.3 New and modified beamlines

The scientific considerations of Section 2.3 have resulted in a set of proposals for new or modified beamlines responding to new scientific challenges. Some require extreme focusing, whereas others, with equally innovative and exciting topics (coherent diffraction imaging, clinical radiotherapy…) have different, but stringent requirements. A strong instrumentation development programme will underpin these scientific advances. Discussions in-house and with external users have led to the following list of projects, summarised in Table 1 (in an arbitrary order), comprising programmes for existing beamlines and instrumentation as well as proposals for completely new beamlines. Advice from the SAC and the Users' Meeting has been sought (and is continuing) on the priorities and choices to be made from amongst these projects. These beamlines are discussed in more detail in Annex 3.

Table 1: New/upgraded beamlines under consideration

Sub-micron focus beamline for coherent diffraction imaging
Beamline developed for clinical protocols in radiotherapy on human brain tumours
Analytical phonon spectroscopy in advanced materials with micrometre spatial resolution (~ factor of 50 improvement compared with an existing inelastic scattering beamline)
Time-resolved absorption and emission spectroscopy with picosecond resolution
Nano-probe energy dispersive X-ray absorption
Soft X-ray beamline for high resolution resonant inelastic scattering and photoemission for the 0.4 – 1.6 kev energy range
Materials science at extreme conditions (including 30 T steady-state magnetic fields and extreme pressures)
Long (~120m) nano-probe beamline and associated laboratories for imaging, spectroscopy and scattering
Long (~120m) pinhole ultra-small-angle X-ray scattering beamline
Time-resolved diffraction beamline for laser pump / X-ray probe experiments
Micro/nano-X-ray diffraction: (canted) beamline branch on existing micro-diffraction beamline
Scanning hard X-ray photoelectron microscopy beamline (~120m)
Energy dispersive beamline for Engineering Materials Science
Coherent diffraction imaging facility for biological samples with ultimate spatial resolution of ~ 20 nm.
Massively automated sample screening integrated facility providing a set of linked MX data collection platforms for the screening of diffraction samples
Small angle X-ray scattering (bending magnet) beamline dedicated to functional biology and applied soft condensed matter research

New and modified beamlines - total estimated cost: 92 M€

4.4 Instrumentation development and beamline support

4.4.1 Introduction

The scientific advances described in Section 2 are only possible if a strong instrumental development programme is pursued as a global effort towards new hardware and new methodologies for integrating mechanics, electronics, metrology, optics, software and computer assistance in new concepts in instrumentation. ESRF is already engaged in this effort in a balanced approach between new developments and support to the beamlines. This effort has already produced innovative instrumentation with benefit to facilities worldwide.

The creation of a Partnership in Synchrotron Radiation Instrumentation, between European SR centres and universities, would be a most effective action to ensure a consistent development at the European level. The focus of such a centre would be on instrument integration and on the full use of new nano-technologies, an area in which Grenoble is one of the most active actors. Instrumentation of the future will involve a high level integration of technologies, where detectors and sample positioning systems, for example, will not be independent components, but will be linked together in a common, dynamic instrument framework. A European partnership should also have a valuable role in the training of scientific, engineering and technical staff to develop and operate advanced SR instrumentation.

4.4.2 Optics

ESRF has become a world leader in the design and construction of highly efficient and stable X-ray optical elements. Future efforts on X-ray optics will be closely linked to the many nano-focusing projects and to future long beamlines. The availability of adequate optics for the most highly demanding experiments in various scientific areas is vital. The goal for future optics is to get as close as possible to the fundamental limits such as the diffraction limit for focusing, by systematically reducing all imperfections of real materials.

Several key items have been identified, where improvements will be mandatory to cope with future needs:

- stable and reliable nano-focusing optics for long beamlines.
- wave front and coherence preservation.
- heat load and radiation resistance.
- sufficient availability of optical elements.

Significant progress in both the fabrication and the characterisation of optical elements is required to achieve these goals. It is mandatory, however, that the technical work is complemented by a theoretical understanding of the properties of the optical device in question. In view of the future challenges in the field of X-ray optics, and in addition to general upgrades of instrumentation, the following dedicated projects and initiatives are proposed:

- Development and fabrication of reflective X-ray optics (Kirkpatrick-Baez (KB) mirrors) producing focal spots down to 20 nm. In this, the accumulated know-how in the design and the operation of curved graded multilayers and the present upgrade of the ESRF multilayer facility will be crucial and important assets.

- Development of a surface finishing device (Ion Beam Figuring) coupled to *in situ* X-ray metrology. This technology will allow the correction of optical surfaces with figure errors below the µrad level and is therefore mandatory for nano-focusing KB optics. The feasibility of this concept has been demonstrated by the prototype machine under development.
- Development of coherence preserving optics operating under high heat load and radiation impact of the white beam. Both crystal and multilayer based optical elements and related cooling schemes have to be optimised to maintain the wave front quality. Diamond crystals will play an essential role for these applications. Their improvement will have to be pushed in collaboration with industrial partners. This project requires access to a dedicated insertion device test beamline.
- Collaborative development and fabrication of transmission optics (compound refractive lenses, Fresnel zone plates, waveguides, etc.). So far, these devices were purchased or obtained through individual collaborations with external institutes. Direct access to the development of such elements could be made by the installation of a dedicated facility as an integral part of a European Nano-Science Centre.
- Development of theoretical tools describing diffraction limited X-ray optical systems. Theories and codes based on wave propagation will be necessary to provide the basis for design and fabrication.
- Development and upgrade of metrology tools. These are essential to analyse the results of the fabrication processes and to improve them, to study the influence of mounting and bending crystals, mirrors and multilayers, to position optical elements in the beam and to detect vibrations and/or thermal degradations. *Ex situ* evaluations will use upgraded instruments in the ESRF optical metrology laboratory. *In situ* studies will be carried out at the Optics Beamline BM05 whenever possible, otherwise, according to present plans, using the undulator source beamtime that will become available on ID06 for optics tests.

It has to be stressed that the above items are strongly interlinked. The overall budget envelope is difficult to estimate since part of the projects will crucially depend on the active participation of external European partners.

4.4.3 Nano-manipulation

The characterisation of samples at the nanometre scale will play a central role in science, raising new problems and new challenges. One of the major difficulties to be overcome will be the recognition and handling of the samples and their manipulation and modification in real time. These problems are at the limits of optical microscopy, while electron microscopy can electrically charge the samples. Pre-alignment could become a very cumbersome operation, while the analysis of free standing samples will be hindered by the electrical charging problems induced by the X-rays. It is necessary, therefore, to envisage a new approach to manipulation and operation at the nano-scale. Scanning Probe Microscopes (SPM) are extensively used in nano-technology to see and manipulate samples of nanometric size, but their application in real time under X-ray beams is just beginning. Nevertheless the reduced size of SPMs and their limited cost makes them ideal for use on SR beamlines, providing new tools for visualising, positioning and manipulating nano-samples.

To cope with the beamline requirements a nano-technology platform will be developed. This will contain a nano manipulation environment of scalable nano-tools able to pick, hold, orient and place nano-objects in synchrotron X-ray beams in order to analyse their properties. These nano-tools will be controlled by an augmented and mixed reality interface providing “touch” feedback associated with audiovisual rendering, the creation of virtual nano-scenes being achieved via a simulator. The realisation of this project requires the integration of many engineering and scientific areas. Given the variety of techniques involved, the project will need the involvement of a number of external specialist laboratories.

4.4.4 Detector development

Major gains in terms of data flow will come from improvements in X-ray detectors. Detector development is of major importance to all SR sources; detectors are generally recognised as the weak link in the modern use of SR. Developments in partnership with European centres must be focused on large area detectors (innovative pixel detectors, silicon drift-diodes avalanche photo diodes and gas filled detectors). The availability of large detector arrays will allow experiments to be performed up to 1000 times more efficiently than is possible with today’s technology: this applies, for example, to fluorescence detection, inelastic X-ray scattering and small angle scattering including microbeam small-angle and wide-angle scattering experiments using a single detector. Such detectors will allow the study of samples that are currently too small, too diluted or too difficult to produce in the required size and shape. Most importantly, however, new X-ray detector arrays offer the possibility of generalised dynamic studies, with the development of correlation and auto-correlation techniques, providing gains of at least two to three orders of magnitudes.

Auto-correlation fluorescence techniques, using a large collection angle and good angular resolution will push time resolution into the microsecond range, allowing dynamical studies of solutions of large macromolecules and of dense gases. This will have a major impact on scientific areas including new materials, self-assembling processes of nano-structures in soft matter, the slow dynamics of proteins in “real” conditions and of systems off thermodynamic equilibrium (with the increasing interest of nano-objects there is a parallel increase in studies of the fluctuations around equilibrium thermodynamic points). For these investigations new detectors are essential.

When analysing in detail the requirements for detectors, it becomes clear that no currently available detector answers all the demands. However, it is also true that the technology required largely exists and that the effort and investment needed is rather in detector development than in detector research. Development is needed on a number of different systems:

- Hybrid pixel detectors: this technology was developed at CERN during the nineties and is implemented on a large scale at the LHC experiments. Various projects have started in Europe to use this technology at synchrotron sources, notably at the SLS (PILATUS) and at the ESRF (Medipix).
- Silicon drift diodes: this would give a few orders of magnitude increase in the efficiency of spectroscopic experiments. This technology has been pushed very

actively by the space research community and large systems are already orbiting in space.

- Monolithic, multi-element silicon avalanche photodiodes: these are for fast timing and time-resolved applications. A nanosecond area detector with a spatial resolution of a few hundred microns would clearly enable unprecedented research. Discussion with industry and other partners (SPring-8, APS, DESY and KEK) are at an advanced stage.
- Fully parallel readout CCDs: to allow a breakthrough in the field of time-resolved high spatial resolution (~1 µm) imaging. Again the technology is available and mature.
- Gas filled detectors, especially for soft condensed matter applications, with the possibility of reaching a spatial resolution below 100 µm and time resolution of about 1 µs.

Micro-electronics design should be further developed at the ESRF; this does not require a full micro-electronics design laboratory, but rather the competence to speak at an expert level with outside designers.

The total budgetary investment necessary for instrumentation development is difficult to estimate precisely at the present stage. The cost estimates for the beamline refurbishment and construction projects described in Section 4.3 already make some allowance for instrumentation development costs. It is clear, however, that research and development programmes are essential to ensure the proper upgrade and exploitation of the new beamlines.

Research and development programmes on detectors, X-ray optics, sample positioning and environment issues - estimated total cost: 30 M€

4.5 Computer infrastructure

The new and refurbished beamlines, equipped with high-performance detectors, will produce an enormous data flow. Already, with existing detectors and data-rates this is creating problems. Depending on the particular beamline we estimate data rates of at least a factor of 1000 higher than today. This calls for a new data communication network able to transport the data from the detectors to the storage systems, high performance computer clusters to process the data, and state-of-the-art software packages for data handling. The new data communication network, based on currently emerging technologies, will provide at least two orders of magnitude higher bandwidth than Gigabit Ethernet. Specialised data transfer software, like GridFTP, may further boost transfer speeds to several GigaBytes/second. The data processing power must allow on-line data analysis for rapid and accurate data interpretation such that feedback loops can be implemented to adopt on-the-fly changes in the data acquisition strategy. It will be necessary to create a computer laboratory providing the space, electricity and air conditioning power to house storage and backup facilities with PetaByte capacities and computer clusters of several hundred nodes.

A major effort will be made on the software side, by installing existing software packages and/or by developing them jointly with other research laboratories, in particular with the upcoming national light sources. The subjects to be tackled cover a wide range of functionalities from sample preparation to data analysis, some of them being:

- European proposal management system: for the common submission and processing of research proposals for synchrotron light sources.
- Laboratory Information Management Systems (LIMS): for tracing the sample preparation, linking it to the proposal and to all experimental data in a consistent manner.
- storage virtualisation, implementing a global name space rendering the access to the data independent from the underlying hardware.
- GRID-enabled data access: implementing authentication, single sign-on, remote access to data and compute resources, GridFTP, GRID portal.
- common data format with normalised metadata: allowing the exchange of data sets between synchrotron laboratories and paving the road for future archiving policies.
- real-time collaboration tools: electronic white boards, video conferencing, electronic notebooks.

Computer Infrastructure - estimated cost: 15 M€

4.6 Scientific partnerships

Most of the scientific programmes carried out with synchrotron radiation have evolved to require ancillary experimental facilities connected to and associated with the experiments at the beamlines. This is justified by many factors such as the lifetime of the sample, its size and properties, and often the need to control precisely *in situ* and *ex situ* its functionality with instruments and techniques other than those strictly specific to SR beamlines. In this context, an example is provided by the time used for data collection in protein crystallography which is negligible compared to the time and effort associated with cloning, expressing, purifying and crystallising a protein. The ESRF has responded to this development by contributing to the Partnership for Structural Biology, a research infrastructure housed in the new Carl-Ivar Brändén Building that brings together all the different expertises required for a cutting-edge structural biology programme.

The new and upgraded beamlines and the additional laboratory and office space arising with the Experimental Hall extension and associated laboratory buildings (Section 4.2) will constitute a new and fertile ground for the development of scientific partnerships in specific areas of science. The ESRF is in an excellent position to be a partner and a host for new European Research Infrastructures of benefit to the wide scientific community, at a time when there is a strong focus on European research infrastructures. The model for a scientific partnership proposed here is based in creating the infrastructure (beamlines, laboratory and office space, basic scientific equipment…) which will allow efficient collaborations between the ESRF and external expert groups around specific scientific projects with well defined scientific goals. This scientific partnership will have to provide clear benefits to the scientific partners for its impact in their own science and to the ESRF users who will be able to benefit from facilities and expertise that go beyond the core competence of the ESRF staff. Scientific partnerships which are being considered at present are in soft condensed matter, in cancer treatment and in the application of high magnetic fields. These partnerships could also be considered as important new research infrastructures within the European Research Area.

Soft condensed matter (SCM) represents a research area in which the ESRF user community in universities, research laboratories and industry has expressed a great interest in creating a partnership that links different experimental techniques to the experiments at the beamlines. Soft condensed matter is also an area that can exploit and benefit from the complementarity of performing experiments on the same sample with neutrons and X-rays. The development of a Partnership for Soft Condensed Matter should involve both ILL and ESRF. A SCM partnership on the ESRF-ILL-EMBL site should contain key facilities for polymer synthesis and deuteration, AFM, STM, cryo-EM, NMR and advanced computing, that may not be available in the laboratories of the users. This partnership will depend crucially on the availability of the infrastructure referred to in Section 2.3.1 as the Nano-Science Centre.

Cancer treatment represents one of the world's greatest health challenges. An increasing engagement in cancer research is taking place on the ESRF-ILL-EMBL site. Promising preclinical trials on brain cancer treatment have been carried out at the biomedical beamline, ILL has initiated similar activities, and several of the research activities within the PSB are related to cancer aetiology and cancer gene therapy. The unique variety of research tools (X-rays, neutrons, molecular and cell biology) available on the same site calls for the establishment of a European partnership for cancer research, which will benefit from the proposed developments of the medical beamline.

Pioneering experiments carried out by ESRF and CRG staff in collaboration with scientists from the leading European High Magnetic Field Laboratories (Toulouse, Grenoble, Nijmegen, Dresden) have shown the feasibility of X-ray diffraction experiments under pulsed high magnetic fields (~ 30T), creating exciting new opportunities in magnetism and magnetic materials. The possibility to develop this collaboration into a partnership which will couple the ESRF expertise in X-ray use with those of high magnetic field laboratories is under consideration. The aim is to provide a unique facility with unique scientific opportunities for the users of the ESRF. The ILL is included in these discussions and the possibility of a shared ESRF-ILL facility to produce large DC magnetic fields is also being considered.

The ESRF, in some cases in collaboration with the ILL and the EMBL, sees it as its responsibility to create the local infrastructure which includes laboratory space and basic beamline equipment to host these scientific partnerships between academia, industry and research laboratories.

5. Staffing Considerations and Cost Estimates

The new and challenging instrumentation developments and increased sophistication of the new beamlines, as well as the substantial increase of floor and laboratory space, will lead to a requirement for a modest increase in the number of staff (~25) as compared to that dedicated today to these areas of operation of the facility (~500).

During the five year renewal programme, and particularly during the construction period, a total of 20 to 30 "peak-load" staff will need to be recruited, primarily in the technical, engineering and building/infrastructure areas. For the subsequent operation some small increase in the regular staff complement will be required. The (~10) upgraded beamlines will be more demanding than those currently operational, both technically and scientifically (e.g. advanced scientific projects involving nano-positioning of samples and extremes of sample environment). Consequently, we envisage a need for 10 additional staff to support the User programmes on these beamlines. As shown in Section 4.4, a major effort is required in instrumentation in the widest sense. We estimate that the continued effort in the fields of detectors, electronics, computing, and sample environment will require ~10 new staff. It is also necessary to consider the increased workloads in the areas of safety and administration. Combined with the requirement to service the increased experimental hall and laboratory space (by Technical Services Division), this leads to a further 5 staff.

A serious discussion has been initiated to consider different possibilities for beamline staffing. Collaborations with universities, industry, and central facility laboratories will be investigated as a means of staffing new and existing programmes at ESRF.

The overall cost of these 25 new staff, added to the ESRF's current complement of ~580 staff, is estimated to be about 2.0 M€, depending on the precise qualifications of these new staff members. Taking account of some slight increase in the operation costs of the upgraded beamlines leads to an overall increase of the ESRF's operation budget of about 3 M€. This increase, of order 4% of the ESRF's current budget is very reasonable, given the very significant scientific benefits to be expected from the upgraded source and beamlines.

Precise cost estimates for the upgrades to the accelerator complex and the beamlines and scientific infrastructure presented in the previous sections are not yet available. Here, estimated costs are given for an upgrade and renewal programme which could start in about two years and would run over a period of five to ten years.

Estimated costs are summarised below:

X-ray Source upgrades	50 M€
Beamline upgrades and new beamlines	92 M€
Experimental Hall extension	45 M€
Instrumentation development and beamline support	45 M€
Grand Total Capital Investment	**232 M€**

The detailed financial and personnel requirements for each part of the upgrade programme will now need to be determined so as to harmonise the renewal projects with the ESRF's current Medium Term Scientific Programme and Medium Term Financial Estimates. Funding sources other than direct contributions from the ESRF's Member Countries will also be investigated over the next year. The ESRF upgrade has been included in the list of major European infrastructure projects presented by the ESFRI group to the European Commission (EC) and is being considered for inclusion in the ESFRI European Roadmap for Research Infrastructures.Financial support will be sought as part of future infrastructure initiatives in the context of the EC 7th Framework Programme. We note that current on-going discussions with prospective new Member or Scientific Associate countries are particularly timely since an involvement in the upgrade programme is expected to be of special interest to the scientific and industrial communities of new partner countries.

ESRF Directorate, May 2006

Annex 1

Beamlines available at European Synchrotron Radiation sources

Facility / beamlines	Energy Range	Techniques	Application	remarks
ALBA 3.0 GeV user operation foreseen for 2010				
MX		Diffraction	Macromolec. Structures, large unit cells	
POLUX	80 - 2000 eV	XRMS, XMCD, polarisation dependent spectroscopies	Hard condensed matter, electronic and magnetic prop.	
noncryst. diffraction	6 - 20 keV	SAXS/AXS, microfocus	Life & Material Sciences	
CIRCE	80 – 2000 eV	XPES, ARPES, XAS, XPEEM	electronic structures, “high”pressure photoemission	
powder diffraction	5 - 25 keV	XRD	high resolution powder diffraction, microfocus, high pressure	
X-ray absorption	2 - 30 keV	XAS, XES, XMCD		
X-ray microscopy	"low energy" BM	microscopy	biological studies within the “water window”	Bending magnet
ANKA 2.5 GeV, operational since 2003				
DIFF	6 - 20 keV	powder diffraction., single cryst. XRD		BM
FLUO	1 - 30 keV	XRF, microprobe, total X-ray reflection fluo.		BM
INE	2.3 - 23 keV	spectroscopy	actinide samples	BM
IR1	IR			BM
LIGA 1	2.3 - 3.3 keV		Mask fabrication, microstructure patterning	BM
LIGA 2	2.5 - 7 keV		Deep X-ray lithography	BM
LIGA 3	2.5 - 15 keV		Ultra-deep X-ray lithography	BM
MPI-MF	5 - 20 keV	XMCD, Surface XRD		BM
SCD	4 - 20 keV	single crystal XRD, MAD		BM
XAS	2.3 - 25 keV	EXAFS, XANES, Q-EXAFS		BM
WERA	80 - 1500 eV	Soft X-ray spectr., XPE,SXMCD, PEEM		Undulator, summer 2005

SUL-X	1.5 - 22 keV	XRD, XRF		Wiggler, 2006
IR2	IR			in 2006
TOPO	white beam BM	topography		BM, 2007
IMAGE	7 - 65 keV	radiography, tomography		SC Wiggler/Undulator
NANO	3 - 30 keV	High res. XRD, anom. scatt., coherent scatt.		SC Undulator
BESSY 1.7 / 1.9 GeV operational since 1998				
ID-02-1	2 - 30 keV		micro-spot	
ID-02-2	6 - 50 keV	X-ray fluorescence, micro-tomography, topography		
ID-03-1	200 - 500 eV			
ID-03-2	6 - 12 keV			
ID-03-3	10 - 35 eV			
ID-04-1	3 - 60 keV	Energy Dispersive Diffraction	Mat. Sci., stress/texture analysis	
ID-04-2	3 - 60 keV	res. mag. scattering, high res. XRD		
ID-05-1	60 - 1300 eV			
ID-05-2	60 - 1300 eV			
ID-06-1a	> 2 keV			
ID-06-1b	> 2 keV			
ID-07-1			PTB metrology	
ID-07-2	20 - 1900 eV		PTB metrology	
ID-07-3			PTB metrology	
ID-08-1	85 - 1600 eV			
ID-09-1	85 - 1600 eV			
ID-09-2	85 - 1600 eV			
ID-10-1	120 - 1700 eV			
ID-11-1	60 - 1300 eV			
ID-11-2	715/786/861 eV			
ID-11-3	60 - 1300			
ID-12-1a	250 - 600 eV			

ID-12-1b	250 - 600 eV			
ID-12-2	1700 - 1800 eV			
ID-13-1	5-180 eV			
ID-13-2	80 - 700 eV	PEEM	nanostructured surfaces, buried interfaces	
ID-13-3	20 - 700 eV			
ID-14-1	4.5 - 17.5 keV	XRD	Protein structure factory	
ID-14-2	4.5 - 17.5 keV	XRD	Protein structure factory	
ID-15-1	85 - 1600 eV			
ID-15-2	85 - 1600 eV			
D-01-1a	95 eV	Lithography		
D-01-1b	1700 - 10000 eV			
D-02-1a	IR			
D-06-1a		Lithography		
D-06-1b	3 - 35 eV		PTB metrology	
D-07-1a1	3 - 35 eV		PTB metrology	
D-07-1a2			PTB metrology	
D-07-1b	1700 - 10000 eV		PTB metrology	
D-07-2	30 - 1800 eV		PTB metrology	
D-08-1b1	200 - 700 eV			
D-08-1b2	200 - 2000 eV			
D-09-2	4.5 - 15 keV			
D-11-1a	20 - 1900 eV			
D-12-1b	4 - 35 eV			
D-13-2	2 - 12 keV	Energy dispersive Reflectometry		
D-15-1a	8 - 120 eV			
D-15-1b	8 - 120 eV			
D-16-1a	30 - 1500 eV			
D-16-1b	4 - 35 eV	circular polarisation		
DAPHNE 0.5 GeV operational since 1998				

DXR1	1 - 7 keV			multi-purpose
DXR2	below 1 keV			multi-purpose
SINDBAD	IR			
DIAMOND 3.0 GeV user operation foreseen for 2006				
phase 1: under construction				
ID2		XRD	Macromolecular crystallography	
ID3		XRD	Macromolecular crystallography	
ID4		XRD	Macromolecular crystallography	
ID6	80 - 2000 eV	XPES, XPEEM, XAS, XMCD, XMLD, microfoc.	nanostructures, MatSci, catalysts, magn. materials, Surf/Int.	
ID15	20 -100 keV		earth, planetary science, MatSci, chemistry	
ID16	3.5 – 25 (15 foc.) keV	polarisation dep. techniques, multi-purpose	Materials, Magnetism	
ID18	2 - 20 (5-30) keV	submicron XAS, EXAFS	submicron XAS, MatSci	
phase 2: under design / constr.				
ID22	3.7 - 20 (8 -12) keV	SAXS, WAXS, ASAXS	extreme conditions, fluid flow at high T, p	
ID11	10 - 20 keV	high res. powder XRD		
ID24		microfocus	microfocus MX	
ID19	5 - 20 keV	XRD	small molecules	
B23		XMCD	Life Sciences / Chemistry	BM
I12 JEEP		XRD	Mat Sci, mat. engineering	
I20	4 - 35 keV	XAS / XRD	diluted samples, MatSci	
I07		XRD	MatSci, Surfaces, Interfaces	
DORIS III 4.5 GeV operation as dedicated 2nd generation machine since 1993				
A1	E_c=16.6 keV	EXAFS, high res XANES		BM
A2	E_c=16.6 keV	SAXS high flux	polymer research	BM

B1 (JUSIFA)	E_c=16.6 keV	ASAXS	nano-porous mat., decomp. of alloys, MatSci	BM
B2	E_c=16.6 keV	powder XRD, res. scatt.	MatSci	BM
BW1		X-ray reflect., GIXRD	Liquid Surfaces, monolayers	Undulator
BW2	E_c=15.8 keV	Surface XRD, Hard XPE, micro tomography	Mat Sci	Wiggler
BW3	15 - 2000 eV	X-ray fluo, XPE, ARPE	core level spect. of atoms, molec., clusters, eletr. structure	undulator, grating MC
BW4	E_c=13.6 keV	Ultra SAXS, time resolved	Mat Sci	Wiggler
BW5	E_c=26.0 keV	High Energy X-ray scattering	applications above 60 keV, MatSci	Wiggler
BW6	6 - 21 keV	XRD, anom. scatt., time resolved (ns…s)	MX	Wiggler
BW7			MX	
C		XAS	MatSci	BM
D1		SAXS	Life Sciences	BM
D2		EXAFS	Life Sciences, EMBL	BM
D3			MatSci	BM
D4		XRD	multi-purpose	BM, under refurbishment
E1		XPE		BM
E2		X-ray reflectometer		BM
E4		XAS		BM
F2		ARPE		BM
F3		EDS		BM
G1		XUV		BM
G3		X-ray Imaging	MatSci	BM
I		VUV luminescence		BM
K			MX	BM, three stations
L		micro XANES, SRXRF		
W1		XPE, high res		Wiggler
W2	"high energy"		Mat Sci	Wiggler, under construction, collab. GKSS
W3		ARPE		Wiggler
X1		XAFS		BM

ELETTRA 2.0 / 2.4 GeV operational since 1995				
1.1L			Life Sciences	short ID
1.2L	50 - 1000 eV	nano-spectroscopy, electron spectroscopy		ID
1.2R	FEL	FEL	FEL	
2.2 L	200 - 1400 eV	scanning photoemission microscopy		ID
2.2R	85 -1500 eV	soft XPE		ID
3.2L	20 - 300 eV	microscopy XPE		ID
3.2R	17 - 900 eV	VUV photoemission	surfaces, solid state experiments	ID
4.2	5 -1000 eV	pol. dependent spectr.	circular pol. light experiments	ID
5.2L	5.4, 8, 16 keV	SAXS, time resolved		ID
5.2R	4 - 25 keV	MAD	MX	ID
6.1L	40 - 800 eV	multi	Mat Sci., industrial applications	BM
6.1R	8 - 35 keV	multi	medical diag., radiology	BM
6.2R	14 - 1000 eV		gas phase investigations	ID
7.1	E_c=3.2 keV	powder diffraction	materials characterisation	BM
7.2	120 – 2000 / 2800 -8000	multi	Interfaces, Surfaces, Overlayers	ID
8.1L	4 - 1400 eV	refl., XAS, opt. absorption	electronic and magn. properties	BM
8.1R	35 - 1600 eV	Lithography		BM
8.2		Dichroism		ID
9.1	IR		Imaging, spectr. in IR	BM
9.2	10 - 100 / 100 - 2000eV	XPE		ID
10.1L		micro-fluo		BM, under commissioning
10.1.R		deep-etch Lithography		BM, under commissioning
10.2L	UV	inelast. scattering		ID
11.1R	2 - 25 keV	XAFS		BM
11.2		XRD		ID, under development
PETRA II 12.0 GeV operational since 1995				

		high-res diffraction, NRS		
	14 -150 keV	XRD, powder XRD, coincident Compton		
PETRA III 6.0 GeV user operation foreseen for 2009				
beamline 1 (decision pending)		IXS, NRS		
beamline 2	XUV / VUV			
beamline 3		SAXS/WAXS, microfocus		
beamline 4		micro-, nano-tomography	Imaging	
beamline 5		XRD	Mat Sci	
beamline 6	5 - 30 keV	resonant X-ray scatt., high res. XRD		
beamline 7		Coherent scattering	dynamics, microsecond to second	
beamline 8		BioSAXS, ASAXS		
beamline 9		XRD	MX	
ASTRID 0.5 GeV operational since 1993				
SGM I	30 - 650 eV		Surface Science	BM
SX 700	6 - 700 eV		Surface Science	BM
XRM	1.5 - 3 nm		X-ray Microscopy, Imaging	BM
MIYAKE	15 - 180 eV		Atomic and Molec. Physics	Undulator
SGM II	12 - 40 eV		Atomic and Molec. Physics	Undulator
SGM III	8 - 150 eV		Surface Science	Undulator
UVI	1.5 - 12eV		CD spectroscopy, Photobiology, UV spectr.	BM
MAX-I 0.5 GeV				
31	15 - 150 eV	scanning XPE		
33	15 - 200 eV	ARPE		

41	15 - 200 eV	ARPE		
52	5 - 30 eV	ARPE, luminescence	atomic, molecular physics	
73	IR			
MAX-II 1.5 GeV				
I311	30 - 1500 eV	XPS, XAS		
I411	50 - 1500 eV	XPS, XAS, coincidence spectr.		
I511-1	50 - 1500 eV	XPS, XAS, XES		
I511-3	50 - 1500 eV	XAS, XES		
D611	2.5 - 8 keV	time resolved XRD		
I711	0.8 - 1.6 Angstrom	XRD (single & powder), SAXS		
I811	2.3 - 20 keV	EXAFS		
D811	1 - 9 keV	nano, deep X-ray lithography		
I911-1	1.25 Angstrom		MX	construction
I911-2	1.043 Angstrom		MX	
I911-3	0.7 -2.0 Angstrom	XRD, MAD, SAD	MX	
I911-4	0.91 Angstrom		MX	construction
I911-5	0.907 Angstrom		MX	
D1011	20 - 1500 eV	XPS, XAS, XMCD		
SLS 2.4 GeV operational since 2001				
X04SA MS	5 - 40 keV	XTM, powder XRD, surface XRD	Materials Science	
X05LA Micro XAS				
X06SA PX	5 - 17.5 keV	MAD	MX	
X07MA Lucia	0.8 - 8 keV	XAS, microfocus	MatSci, environmental, cult. heritage	
X09LA SIS	10 - 800 eV	high res PES, ARPE, PED, XPE	electr. and atomic structure of surfaces	
X10SA PXII	6.5 - 20 keV		MX	
X11MA SIM	90 - 2000 eV	PEEM, XMCD		

SOLEIL 2.75 GeV user operation foreseen for 2007				
SIRIUS	2 - 10 keV	GIXD, GISAXS, resonant anom. scatt.	soft interfaces, nanostructures	2008
LUCIA	0.8 - 8 keV	micro XAS, XRF	microprobe	2008
SMIS	IR		micro spectroscopy	2006
AILES	IR		ultra-high resolution	2007
ID3C			high pressure studies	
PLEIADES	10 - 1000 eV		spectroscopy of atoms/clusters/diluted samples	2007
DESIRS	5 - 40 eV		atomic, molec. systems, very dilute	2007
CRISTAL	3 - 25 keV	XRD	crystallography condensed matter	
DEIMOS	350 - 2000 eV	XMCD XMLD		
GALAXI	3 - 12 keV	IXS, high energy XPE	electronic structure / excitations	
TEMPO	50 - 1500 eV	rapid XPE, XMCD, pump-probe	dynamics of electronic and magnetic properties	2006
PROXMA 1/2	5 - 15 keV	MAD/SAD.XRD	MX	2006
SWING	5 - 17 keV	SAXS/WAXS/GISAXS/anomalous scatt.	soft condensed matter	2006
ANTARES	10 - 1000 eV	ARPE, PED	electronic structure, Fermi surfaces	
MICROFOCUS	50 - 1500	RXMS, XRIS, X-PEEM		
SIXS	5 - 20 keV	GIXD, GISAXS	surfaces, interfaces	
CASSIOPE	10 - 1000 eV	ARPES, spin resolved spec, resonant spec.	electronic, magnetic structures	
ODE	3.5 – 25 keV	XAS in scattering energy dispersive mode	magnetic scattering	BM beamline
MARS	3.5 – 36 keV		radioactive matter	BM beamline
DISCO	60 – 700 nm	VUV circular dichroism	MatSci, Biochemistry	BM beamline
METROLOGY	10 eV – 15 keV			BM (3 branches)
SAMBA	4 – 40 keV	XAS	MatSci, Biomaterials	BM beamline
DIFFABS	3 – 23 keV	XRD, XAS	MatSci	BM beamline
FEMTO				

Annex 2

Report on discussions at ESRF Users' Meeting of February 2006

The ESRF Users discussed the ESRF Long Term Strategy in detail at the 2006 ESRF Users' Meeting, held at the ESRF on February 6 and 7 2006. The LTS was presented to the Users by the ESRF Management and via the draft document "New scientific opportunities at the ESRF" published on the ESRF web-site. The Users, together with the ESRF scientists, convened in seven parallel discussion sessions, identified by specific scientific areas and use of synchrotron radiation, and organised by the members of the Users Organisation (UO) together with ESRF scientists. The discussions were focussed on the medium and long term evolution of the ESRF, and how the Users perceive the ideas contained in the draft document. To this end the following issues were proposed as topics for discussion:

- priorities of the proposed scientific and technical developments.
- collaborations necessary to fully develop new beamlines, involving (for example) in-kind contributions from experts in areas other than those where specific expertises are present at the ESRF.
- science-driven or technology-driven proposals from the communities that could develop into a partnership including the ESRF.
- priorities for further development of the ESRF support infrastructure.
- ESRF's role in the context of the upcoming European SR Sources.
- changes in the ESRF use once the new European SR sources will become operational.
- issues not included or fully considered in the LTS paper.

These topics were discussed in the different sessions with different emphasis and priorities. Each discussion leader provided a short report which is presented below.

From the reports it is possible to identify a number of common aspects. In general there is enthusiastic support for the ideas presented in the document "New scientific opportunities at the ESRF". It is clear that each community favours certain aspects of the upgrade but in general one can conclude that:

- the scientific case successfully touches all the areas reflecting the evolution of the scientific interests of the communities using the ESRF.
- the proposed technical developments on the machine, the beamlines and the infrastructure are generally supported.
- increasing emphasis is given by the Users to support major developments in the scientific infrastructure ancillary to each specific synchrotron radiation experiment. In this respect many Users are ready to engage themselves in such endeavours, both via scientific partnerships and long term projects.
- important developments on sample environment and positioning issues are considered of primary importance for many field of synchrotron based science.
- detector developments and on-line real-time data analysis are areas which require immediate attention for an efficient and productive scientific programme, especially in those areas where data acquisition flow is already

very high and expected to increase: examples are imaging and tomography beamlines and macromolecular crystallography beamlines.

Report on the discussion held during the parallel session of the High-Resolution and Resonance Scattering group: Claudia Dallera (UO), Rudolf Rueffer (ESRF)

The main results from the discussion of the High-Resolution and Resonance Scattering group, which took place on the first afternoon of the ESRF 2006 Users Meeting are summarised below. Beamlines ID16, ID18/ID22N, ID26 and ID28 belong to this group.

There is a general consensus that the highest priority should be given to the improvement of the detection capabilities. This is important both in the frame of medium and long term strategies from the point of view of the development of new detectors (which could be organised in the frame of large collaborations) and with the goal of increasing the collection angle. In fact, the speciality of this group is inelastic X-ray scattering, which is a technique with low count-rate experiments, and efforts towards increasing the collection angle by having more efficient spectrometers with a large number of crystal analysers are already underway.

The increase in ring current will of course also be very beneficial to increase the detected intensity. In order to further improve the already good beam stability, interest has been expressed in the implementation of the continuous top-up injection mode that would result in a constant heat load on the optical elements. Of course some experiments will need to gate out the data collected at the injection instant due to the sudden variations that occur to the beam.

There is general consensus that very good support is received from ESRF beamline staff and infrastructure. A suggestion was given that a more user-friendly interface to the beamline control would allow users to become independent more rapidly, thus partly releasing the beamline staff from their local contact duties and improving the overall efficiency of the experiments.

A point requiring a major effort in the future is felt to be the collaboration on sample environment facilities: it has been suggested that an efficient procedure could be to develop some particular parts of the sample environment at the home institution, and then requesting support for (e.g.) interfacing the sample setup to the instrument at the beamline. This would minimise incompatibilities and difficulties during the experiment.

Report on the discussion held during the parallel session of the Materials Science Group: Alain Lodini, Ake Kvick (ESRF)

Synchrotron X-ray studies at the ESRF have already produced world leading research in materials science and engineering. The ability to successfully deliver the best research will need investment and commitment to providing facilities to support engineering research. The foundation of the FaME38 facility has been a valuable first step in this process. Areas of materials science research in which synchrotron X-rays play a leading role are those identified as major socio-economic drivers, and contribute fully to the formation of a pan-European knowledge-based economy.

- Energy. The production, transport and storage of energy are a critical challenge for the entire European economic area. The production and use of hydrogen as a fuel (the hydrogen economy) is also a developing research area where in-depth materials research is required. Predicted future energy requirements indicate that there will be a need for new nuclear reactor technologies. These will require the characterisation of new materials and measurements of stresses under operating conditions to ensure safe plant life.
- Transport. This is linked to energy use in the development of technologies such as fuel cells for vehicle power. Again, new materials will play an important part in the evolution of future transport technologies, with the aim to reduce the weight of vehicles and so reduce fuel consumption. This applies equally to the automotive, rail and aerospace sectors. New composite materials require characterisation of their internal stress behaviour during loading, for example.
- Healthcare. The ageing population will become increasingly reliant on implants and prostheses for quality of life. New materials technologies including biomimetic coatings and novel methods of drug delivery will require characterisation and performance assessment.
- Environment. New materials are under development for technologies such as carbon entrapment. All industrial sectors face the challenge of increased recycling and minimal disposal of the materials used in their products. Materials for the safe storage of nuclear waste require research to ensure public confidence and acceptance. Sustainable development and the safeguarding of the environment underpin many of the materials developments for the coming decades.

These areas are underpinned by materials research: materials processing, functional materials, smart materials, bio-materials, and a better understanding of traditional materials as part of their incremental improvement. In terms of the provision of support for studies in these areas, synchrotron X-ray sources need to address the following issues:

- The formulation of a clear strategy for the support of researchers in the fields of materials science and engineering.
- The provision of ancillary equipment for *in situ* materials characterisation and environmental simulation, including robotic methods for sample positioning and manipulation, the possibility of performing experiments under harsh and extreme environments and equipment for the support of dynamic experiments.
- The implementation of software tools for easy data analysis and experimental set-up.
- Finally, serious consideration should be given to the provision of a dedicated beamline for applications in materials science and engineering.

The development of international standards is ongoing and will support the broadening of the user base in the use of synchrotron X-rays for materials research.

During the discussion the group endorsed the long-term plans in general and in particular

- the extension of the Experimental Hall;
- the focus on nano-science, extreme conditions and time-resolved studies;
- the addition of laboratory and office space to facilitate long-term projects and long term proposals;
- the recognition of the need for additional beam-line capacity for high-pressure and time-resolved studies.

The group also stressed the unique niche of high-energy research at the ESRF as being of particular relevance to the materials and engineering community. The group did not see any comparable alternatives provided by the emerging synchrotron facilities (although PETRA-III might provide some relevant facilities). This should be highlighted in the long term plans. The group endorsed activities on large volume presses.

The value of FAME 38 as a starting point for further engineering activities was recognised. It was suggested this to be a nucleation point for the development of Partnership for Materials Science. A suggestion was given that a broader community should be contacted under the leadership of Prof. A. Lodini to obtain further information on the needs and interest for the formation of such a partnership.

Report on the discussion held during the parallel session of the X-ray Absorption and Magnetic Scattering Group: Nicholas Brookes (ESRF)

The intensive discussion during the parallel session converged to the following conclusions:

- The energy region below 10keV is of significance to this community since the important absorption edges are in this energy range.
- Sub-micron spot sizes are not of as much importance as in some synchrotron radiation research fields but still could be an important factor for a variety of applications.
- High magnetic fields, low sample temperatures, high pressure etc. are felt to be an important area of development for future applications.
- The community favours more involvement/collaboration with external scientific bodies, institutes, universities etc. organised as partnerships and long term projects driven by scientific objectives.
- Even with other synchrotron facilities providing, in principle, comparable performances, it is thought that the users will still come to the ESRF. The type of service provided is important in this aspect. The idea that the ESRF provides a “complete package” is of major importance. Local support, infra-structure and local expertise are important factors which give scientific and technical strength to the ESRF.
- More infrastructure support for sample handling and local characterisation is highly demanded.
- Beam stability is a very important parameter for the future and must be kept/improved compared to present performances.

- Topping-up was discussed with varying opinions. Advantages and disadvantages are identified, the important point being not to degrade the beam stability.
- The group is mainly interested in high magnetic fields, high pressures and low temperatures and understands that these developments (i.e. for what concernes high magnetic fields, molecular magnetism studies would benefit from fields up to 50 T) would require a stronger user support and therefore encourages an increase in manpower.
- As a final remark it should be noted that there is a general feeling that there will be an expanding community of users and more experiments approved at ESRF. The group is convinced of the need for maintaining the ESRF as a leading facility.

Report on the discussion held during the parallel session of the X-Ray Imaging Group: Laszlo Vincze (UO), José Baruchel (ESRF)

The first part of the “X-ray imaging” parallel session featured three short talks reporting on the various technical/methodological developments at various X-ray imaging beamlines, including an overview of the evolution of BM05 towards imaging and coherence experiments by E. Ziegler, a report on the use of diamond for X-ray optical applications by J. Härtwig and a summary on the developments of infrared microscopy at ID21 by M. Cotte.

The subsequent discussion was introduced by two general reports on the nanofocusing coordination at the ESRF by J. Susini and on the future evolution of X-ray imaging within the Long Term Strategy frame by J. Baruchel.

These talks and the subsequent discussion identified the highest priority developments and needs for the X-ray imaging community that are associated with the following areas:

1) Evolution of the biomedical work: improvements in biomedical (functional) imaging and developments in clinical radiotherapy within the framework of large collaborations for this type of cancer treatment.
2) Further evolution in microtomography should satisfy the following requirements:
   - more access for users
   - better spatial resolution down to nanoscopic levels
   - better temporal resolution

A very important issue is the further development of 2D-detectors for various needs, which are still too slow when high (spatial and temporal) resolution levels are required, or to perform functional imaging. Further developments of X-ray detectors as well as other components, such as X-ray focusing optics, could be performed within the framework of large integrated European projects, with a potential coordination by the ESRF. Concerning the developments in nano-imaging, various recommendations emerged, including:

- project meetings between beamlines of various experimental groups (e.g. ID11, ID13 and ID22M)

- regular organisation of international nanoscience meetings
- setting up a central database for various nanofocusing optics (CRL, Fresnel zone plates, mirrors, crystals etc.).

Combination of microanalytical techniques include:

- Microtomography combined with various spectroscopic techniques (e.g. XRF/XRD/XANES/EXAFS) should be pursued with nanoscopic resolution. In this respect the stability of micro- (nano-) EXAFS represents a serious problem even on the micrometer scale, which should be taken into account during the developments of micro-spectroscopy beam lines.
- Combination of X-ray imaging with electron microscopy, which would be very useful for nanoimaging and sample visualisation when optical microscopy reaches its theoretical limits of resolution.

Further developments are needed in the field of data evaluation for phase-contrast imaging techniques. A task-force should be created for improving the coordination among phase-retrieval techniques developments. On-line data reduction/evaluation in general is an important issue for imaging and scanning micro-spectroscopy, and its development should be further pursued.

Oversubscription is a serious issue at imaging beamlines, therefore the increase in the number of end-stations will be a positive development. The possibility of external staffing via partnerships should be considered, possibly via 7th framework EU-projects.

Report on the discussion held during the parallel session of the Surface and Interface Science Group: Chris Lucas (UO), Joerg Zegenhagen (ESRF)

Christian Mocuta (ID1) gave the first presentation showing examples of micro-beam diffraction studies of nanotubes and Ge pyramids on Si and coherent X-ray diffraction measurements from Au microcrystals. Joerg Zegenhagen then summarised the group activities on beamlines ID1, ID3 and ID32. Olaf Magnussen (University of Kiel), gave an excellent introduction to the electrochemical interface and then described some recent results concerning Au homoepitaxy, hydrogen evolution on Pt and liquid mercury electrodes.

The talks were followed by detailed question and answer sessions from a packed audience. The ESRF long term strategy (LTS) document was summarised by Chris Lucas as a lead-in to the discussion session where the questions summarised at the head of this Section were addressed.

This generated a great deal of discussion as to the potential limitations in studying single nanoparticles and exactly how long a beamline would have to be in order to have sufficient space around a sample. The highest priority for infrastructure support was deemed to be detector development. It was pointed out that there appeared to be a gap in the accessible energy range of synchrotron sources in the range 20-50 keV and the ESRF could fill this gap. Looking at the future it was noted that the LTS describes a strategy that would be governing experiments performed in 5-10 years. It was thought that consultation, not only with the synchrotron community but also with outside communities (the electronics and chemical industries were given as two examples), would be very important in forming such a research strategy. This matter was raised at the question and answer session with the ESRF Directors on the following day.

Report on the discussion held during the parallel session of the Soft Condensed Matter Group: Tanja Asthalter (UO), Christian Riekel (ESRF)

The first part of the session was devoted to ongoing and planned extensions of several Soft Condensed Matter beamlines.

Ongoing projects: Recent developments and the strategy of the SCM group and its associated beamlines for the next years were presented by C.Riekel:

- The ID13 beamline will start commissioning its nanofocus extension, which will be located at the outside of the experimental hall, by the end of 2006. The aim is to reach spot sizes of 50 nm and smaller. For the time being the new nano-branch will operate alternatively with the existing micro-branch, which will provide beam sizes of about 1-5 µm and provide more flexibility for SAXS/WAXS experiments. The micro-branch will also continue providing the possibility for combined micro-Raman and micro-SAXS/WAXS experiments.
- The FP6 SAXIER project started in December 2005. It aims at developing high brilliance SAXS applications at several European synchrotron radiation laboratories (spokesman D. Svergun, EMBL Hamburg). The ESRF beamlines ID13 (Riekel) and ID10B (Konovalov) participate in several work-packages on nanobeam SAXS/WAXS, combined microRaman and micro-SAXS/WAXS as well as microfluidics developments. Other participating groups are from Soleil, Daresbury and Graz/Elettra.

Long-term strategy: The following projects are foreseen:

- A separation of the ID13 nano- and micro- branches into independent beamlines by a Troika-type optics or canted undulators in order to reduce the high demand on both branches.
- A bending magnet SAXS/WAXS beamline in order to provide high throughput solution scattering capabilities for protein crystallography. This beamline is also proposed for soft condensed matter experiments not requiring the highest brilliance but the possibility of more systematic and high throughput R&D (e.g. applied and industrial research).
- A pinhole USAXS beamline extending the time-resolved capabilities of ID02 to smaller Q-values. Applications could for example be in aggregation studies on large polymeric complexes, jamming transitions in colloidal systems or particle aggregation in spray pyrolysis experiments. The design of ID02 aims at a beam splitting in analogy to the one planned at ID13, such that the current SAXS pinhole camera and the USAXS branch can coexist (presented by T. Narayanan).
- C. Riekel stressed the importance of developing a Soft Condensed Matter Partnership together with external user groups. As an example he mentioned

the possibility of developing highly complex sample environments outside the constraints of daily beamline operation.

Report on the discussion held during the parallel session of the Macromolecular Crystallography Group: Pedro Matias (UO)

A major part of the session was dedicated to some aspects of the ESRF Medium and Long-Term Strategy that have impact on the Macromolecular Crystallography community. One particular point of discussion was the need for an MX-dedicated beamline using short wavelength radiation (~0.33Å) for data collection and it was emphasised by some speakers that the 'new' ESRF will be in a unique position to take advantage of the properties of short wavelength radiation for MX experiments.

The presentation by Elspeth Gordon on the long term strategy for data collection, where users may not need to travel to the ESRF to carry out experiments, elicited much interest amongst the audience and a wish was expressed that the same facilities that are currently available to industrial users (i.e. MXpress) should be made available to academics for the more trivial projects. As pointed out by Sean McSweeney, an extension of the MXpress scheme to academic users would not only entail a higher number of beamline staff but also a different hiring profile, more oriented to technicians rather than scientists. Sine Larsen mentioned that the higher staff expenses might be balanced by the reduced need to pay for MX users travel and accommodation. A final item that received much interest was the MASSIF system, for which it was decided to request more details and a tentative schedule for its implementation from the ESRF Directors.

Annex 3

Proposed new beamlines and beamlines to be refurbished

01: Focus on Coherence

Summary

The aim of this project is two-fold: (i) to exploit micron and sub-micron focused X-rays for the study of local properties of nanostructured materials and (ii) to use the beam coherence to perform coherent diffraction imaging of nanosized crystals or non-periodic objects. In the case of nanometer-sized objects, the coherent flux needs to be increased by focusing optics, combining a small focus with the (reduced) transverse coherence of the beam. The planned extension of ID01 will be based on new undulators, a new tandem monochromator and a stable setup by mounting the diffractometer and the focusing elements on the same support table in the experimental hutch.

Scientific case

The progress in nanoscience and nanotechnology asks for tools to characterise the structure of objects both on the mesoscopic and atomic length scale. One big challenge in this field is the investigation of *individual* nanostructures, which is important to quantify variations in self-assembled structures and to correlate these variations with the particular nanostructure location. This will be increasingly important for nanostructures embedded into electronic devices.

Using a sub-micron focused beam, *real space* mappings will be combined with fluorescence microscopy and diffraction experiments in *reciprocal space* to obtain strain, size and chemical information. Combined with anomalous scattering they are applied for analysis.

The coherence of the beam will be used to study the structure of periodic and non-periodic objects on nanometer length scale by Coherent X-ray Diffraction Imaging (CXDI). The novel technique of phase retrieval by Fourier over-sampling leads to the *direct* determination of strain and shape in a single object, with resolution in the nm range.

The novel techniques will play an important role in the understanding of the structure, fabrication and functionality of nanomaterials. Applications include the investigation of surfaces and interfaces, extended defects, granular materials, self-assembled and semiconductor nanostructures, etc.

Technical aspects

A new tandem monochromator is needed to improve the beam stability and to obtain the low divergence beam needed for large transverse coherence lengths and sub-micron focusing. Focusing optics and the diffractometer will be placed on the same vibration-damped support. A two-dimensional detector will be decoupled from this setup and positioned by a heavy-duty robot arm.

The new setup will fit into the experimental hutch without the need of removing existing equipment. The SAXS option at ID01 can be used for coherent diffraction imaging in the forward direction with adaptable resolution due to variable detector-to-sample distance of up to 7 m. In the case where CXDI uses the "old diffractometer set-up", ID01 will be especially well suited for high coherence applicationsdue to the low energy x-rays available in a windowless setup.

Estimated cost and staffing

The budget needed for the project is about 1M€.

During the design and construction phase, an extra engineer will be needed.

For the construction and commissioning of the new setup, as well as for the development of the techniques (microdiffraction and CXDI, with the option to use anomalous scattering) a postdoc position is needed.

Existing or new BL/ section/length/canted undulators

The low-ß section of ID01 will be refurbished by two new U35 and one U42 undulator, all having the option of a small gap of 10 mm to increase the flux and to use the first harmonics of U42 for low energies. This undulator replacement has already been planned by the machine division independently from the project.

Timescale

We plan to install with first priority the new monochromator in the summer shutdown 2008. The design of the vibration-damped support table, diffractometer, and detector mounting will be made in parallel. The installation for these parts could be foreseen for the winter shutdown 2008/2009, followed by 2 months of commissioning.

Possible location

Since there is sufficient space in the experimental hutch of ID01, no changes are required, with the exception of two larger doors.

Computer needs

The size of the recorded data is expected to be very large and the storage and processing of these quantities of data requires well suited high-end computing equipment.

Detector needs

Two-dimensional detectors with high spatial resolution, high dynamic range, high efficiency and reduced readout time are crucial to achieve the scientific goals.

Other needs concerning support groups

The partnership with external institutes, specialised in the fabrication of optics/nanofocussing devices, implies the existence of a group active in these technologies at the ESRF.

Associated laboratories

The project *Focus on Coherence* would highly benefit from the propositions made by the Soft Condensed Matter and X-Ray Imaging groups in the project “Long nanoprobe beamline (and associated laboratories)”, in particular the **European Centre for the production of nano-optics devices** (see proposal 08).

02: Clinical Protocols in Radiotherapy on Human Brain Tumors

Summary

We propose to implement at ID17 Phase I (patient safety) and Phase II (effectiveness of the treatment in a selected population) clinical protocols in radiotherapy to check for the efficiency of synchrotron radiation therapy on human brain tumours. Preclinical results achieved by ID17 users are internationally recognised to be at the cutting edge for treating these diseases. The ESRF is the unique place in the world where such trials will be possible in the next years.

Scientific case

For many years, the ID17 Medical Beamline has developed innovative preclinical research in radiotherapy in collaboration with different groups of users. Two programmes, namely the Microbeam Radiation Therapy (MRT) and the Stereotactic Synchrotron Radiation Therapy (SSRT) provided exciting results paving the move towards clinical trials (Phase I: patient safety and Phase II: effectiveness of the treatment).

Both research programmes are presently targeting brain tumours, either in infants (MRT) or in adults (SSRT) for which standard clinical therapy is only palliative.

The ESRF is presently, and will be in the near future, the unique SR facility in the world where clinical trials in radiotherapy will be possible. This is due to the presence, on the same site, of a beamline with adequate spectrum and X-ray fluency, of bio-medical infrastructures and of strong collaborations with hospital teams.

Technical aspects

The technical needs are different for the two programmes, even if expertise and developments in radioprotection, treatment planning, and beamline medicalisation are needed in both cases.

MRT. The treatment has to be performed with a spatially fractionated (microbeams 25 - 50 µm width) intense (dose rate > 1000 Gy/s) pink beam (mean energy ~ 100 keV).

<u>Phase I on peripheral tumours</u>. In order to verify the safety of MRT, a Phase I protocol would be performed on peripheral (arm, hand) tumor metastasis. This solution does not necessitate building new hutches. It would provide preliminary clues for the evaluation of necessary investments for Phase I and Phase II studies on brain tumours. This protocol would be performed in the present first ID17 hutch and would need the following items: installation of a patient shielding, modification of the present patient positioning system and development of the safety system (based on fast reaction shutters).

<u>Phase I and II on brain tumors</u>. This new protocol would benefit from the technical developments and know-how achieved above.. A new white beam hutch would be required because of the limited space in the present one. New items to be developed include an irradiation room, a patient positioning system for infants, and an upgrade of the safety system.

SSRT. The treatment has to be performed with a monochromatic X-ray beam of about 80 keV, already available at the ID17 satellite building.

Phase I and II. Most of the equipment, i.e. patient positioning and safety system developed for the angiography clinical program can be re-used for this programme. However, a technical upgrade has to be foreseen for assuring the accurate X-ray dose delivery to the patient. Technical developments include the upgrade of the patient positioning system, the implementation of the treatment planning in the beamline control system, the development of a fast slit system for shaping the beam to the target dimensions and the development of attenuators for portal imaging (imaging during irradiation).

Estimated cost and staffing

SSRT and MRT costs are different, however overall costs can be estimated as 2 M€. Moreover, in the clinical phase and in its preparation, a Medical Physicist expert in radiotherapy treatment planning and clinical procedures would be of great advantage for the beamline. He/she could act as a bridge between the ESRF and hospitals and take care of the treatment planning systems.

Existing or new BL/section/length/canted undulators

The present wiggler source meets the flux needed for the clinical trials, when the machine runs at maximum current. ID17 is presently the only beamline at the ESRF with just one insertion device; a second wiggler, with similar characteristics, would open the way to perform preclinical research and clinical trials in radiotherapy at lower machine currents.

Timescale

The definition of the detailed technical aspects for the clinical implementation will be completed in 2005 for SSRT and in the first quarter of 2006 for MRT. The design could then start once funding becomes available.

Possible location

SSRT will be performed in the present ID17 imaging hutch already prepared for angiography clinical trials. A new MRT clinical hutch will be constructed next to the present ID17 MRT hutch in the experimental hall.

Computer needs

Powerful computing resources are needed to prepare the treatment planning, since software based on Monte Carlo simulations is used to optimise the dose delivered to the tumour while sparing the surrounding organs.

Detector needs

In-line, fast reaction dose monitors are needed for MRT for monitoring the microbeams.

Other needs concerning support groups

Strong collaboration with ESRF engineering, computing and safety groups is needed during all phases of the project.

Associated laboratories

A **European Centre for Cancer research**. The **ID17** Biomedical beamline is only one of the laboratories on the ESRF/ILL/EMBL site developing cancer research: additional laboratories include **ID21-ID22** (quantification of high Z elements in cells, bystander effect on single cells), **ID14** (study of cell cycle regulatory proteins, resistance of bacteria to high radiation doses) the **PSB partnership** (study of bacterial and viral pathogens also related to cancer etiology), **EMBL** (carcinogenesis studies via RNA and DNA analysis), **ILL** (Boron Neutron Capture Therapy). Synergic programs could be developed by the creation of an institute through the European Community for funding. Its cost is at least in the 5 - 7 M€ range.

03: Analytical Phonon Spectroscopy in Advanced Materials with Micrometer Spatial Resolution

Summary

We propose to build a high-throughput inelastic X-ray scattering spectrometer, devoted to the determination of elastic, vibrational and thermodynamic properties of materials relevant for applications in fields ranging from biology to nanoscience. The enhanced capabilities of this instrument, in conjunction with powerful and precise lattice dynamics calculations, should reduce typical experiment times from several days down to hours.

Scientific case

Progress in materials research is intimately linked to the utilisation and development of powerful and efficient analytical techniques, aiming at a complete understanding of the materials' structural, electronic and vibrational properties. In view of the current trends towards complex (microstructured) materials, thin film and nanotechnologies, novel approaches to link the microscopic characterisation with the macroscopic properties are indispensable [1]. Traditionally, three different analytical approaches can be distinguished: diffraction, microscopy (imaging) and spectroscopy. Their use and impact in materials research is closely connected to the maturity of the technique and to the time scale in which relevant results can be obtained.

While inelastic x-ray scattering (IXS) from phonons has succeeded to evolve within less than ten years into a valuable spectroscopic tool, its broad application is hampered by the fact that (i) typical experimental times range between one and two weeks, (ii) various applications are still under development and (iii) experimental results are not routinely coupled to powerful computer based theoretical simulations. Nevertheless, pioneering experiments give a flavour of possible future breakthroughs in areas such as superhard and carbon materials [2-5], thin film and surface science [6], and large band gap semiconductors [7]. The development of IXS as a routine tool is highly desirable, since IXS allows the determination of a wealth of elastic and thermodynamics properties, therefore providing critical input for a complete material characterisation.

In order to overcome the limitations of IXS outlined above, important efforts have to be undertaken (i) to couple the experimental results with highly developed and efficient (*ab initio*) lattice dynamics calculations and (ii) to enhance the spectrometer efficiency by at least a factor ten. For single crystal work a properly chosen, restricted set of experimental spectra (along high-symmetry *and* arbitrary directions in reciprocal space) can be sufficient to determine the full phonon dispersion, if the calculations are refined in terms of phonon energies *and* intensities. In a similar fashion it can be anticipated that for polycrystalline samples, the complete single-crystal phonon dispersion scheme can be derived, if IXS spectra are recorded over a large momentum transfer range up to the density-of-states limit.

Technical aspects

Based on the current know-how in crystal analyser fabrication and the expected advances in large area pixel detectors, a compact multi-analyser spectrometer (4 m Rowland circle geometry, equipped with a bench of 25 (75) analysers, and covering scattering angles up to 50 degrees) with adaptable energy resolution (utilising the energy dispersion within the focal spot size [7]) and variable momentum transfer resolution is within reach. Four specific technical items have to be developed, or implemented: analyser fabrication and development, detector development, beamline optimisation and computing infrastructure.

Estimated cost and staffing

Analyser fabrication and development (1000 k€)

A technician with specialisation in optics needs to be fully dedicated to the analyser development program. Alternatively, the analyser production could be outsourced to an optics company.

Detector development (1000 k€)

If we "parasitically" benefit from the development as it happened for Medipix-II, the necessary resources can be supplied within TBS.

Beamline optimisation: high resolution monochromator, focusing optics (750 k€)

The major upgrade program requires the full dedication of one draftsman and one engineer over a period of three years.

Computers and software development (150 k€)

Resources are either available in-house or development/installation can be outsourced.

Existing or new BL/section/length/canted undulators

The project is based on an X-ray source composed of three revolver undulators with optimised performance at 17794 eV and 21747 eV, located on an even numbered ID.

Timescale

2008-2011

Possible location

The project can be based on an even numbered ID-section, either on one of the existing IXS beamlines (ID16 and ID28), or at a newly assigned location.

Computer needs

There are several highly developed and very performing (*ab initio*) lattice dynamics software packages already available, some of which are commercialised. The necessary software developments are therefore restricted to an optimised interface with the experiment, allowing for rapid visualisation and comparison with experiment. In order to perform this in real-time, a PC-based computer cluster is needed.

Detector needs

There are at present intensive research efforts on pixel detectors such as the Medipix II. At present these detectors are based on silicon technology, but projects using GaAs and CdTe have been launched. These latter pixel detectors ensure the complete absorption of photons, even at 25.7 keV, and, in view of the enormous impact of detector developments for all disciplines of science, it can be expected that these detectors will be available in a few years.

Other needs concerning support groups

Analyser fabrication methods have been continuously refined over the past 15 years, and have reached a high level of quality and reproducibility. The production of a large amount of these analysers nevertheless needs further improvements in the processes and the metrology.

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04: Picosecond Spectroscopy

Summary

We propose time-resolved absorption and emission spectroscopy using a pump-and-probe scheme with laser photoexcitation. The separation of the X-ray pulses can be achieved by either a chopper or fast detectors (APD) in connection with wavelengths dispersive X-ray emission spectrometers. We stress the importance of enhancing the time-resolution from currently ~100 ps by a factor of ten.

Scientific case

Time-resolved spectroscopy has revolutionised our understanding of fundamental processes in chemistry, biology and material science. The technique requires a pump pulse that creates a short lived state in the system under study while the decay is monitored with a probe pulse that is applied at a time ?t after the pump pulse.[1, 2] Even though time-resolved spectroscopy is well established using wavelengths in the optical range, many applications call for an element specific spectroscopy using X-ray probe pulses.

The scientific case for picosecond spectroscopy is distinct from the femtosecond realm that will be entered with new X-ray sources such as the X-FEL. While in the latter non-linear processes or coherent atomic displacements in vibrational relaxations will be studied, picosecond spectroscopy addresses the large field of photo(bio)chemistry with non-coherent atomic motions and topics in material science, e.g. magnetic switching and laser-induced phase transitions. Understanding and modeling photoinduced energy and electron transfer in photosynthesis, oxygen transportation and molecular devices such as photonic, electronic, or optoelectronic devices, will greatly benefit from the structural and electronic information gained in picosecond spectroscopy. To name an example, the photochemistry of metalloporphyrins (e.g. (Ni(tpp)L_2] or ($Ru^{II}(bpy)_3]^{2+}$) with their numerous applications as molecular devices is of prime interest because the kinetics of the local coordination at the metal site can be studied selectively by means of an inner-shell spectroscopy.[3] Here, the structural deformations occur on timescales between several hundreds and tens of picoseconds. It is therefore desirable to achieve X-ray pulse widths below 100 ps.

Technical aspects

Building on the expertise in time-resolved diffraction at the ESRF, time-resolved X-ray absorption (XAS) and emission (XES) spectroscopies can be developed. The combination of picosecond XAS with high-energy resolution (?E/E ~ 10^{-4}) emission spectroscopy is novel and has several advantages:

1) The chemical information contained in the emission spectra is complementary to that available from absorption spectroscopy.[4]
2) The small energy bandwidth in the emission detection allows us to better resolve absorption features. This can lead to dramatic improvements in particular for high Z elements.
3) High energy resolution emission detected XAS is virtually background free.
4) Using a wavelength dispersive detection scheme gives large freedom for the selection of the detector. Thus, very fast detectors can be employed in the range of the desired time-resolution giving more flexibility in using the incident X-ray pulses (e.g. pump pulses on every second probe pulse). A chopper will then be used to protect the sample from radiation damage and/or allow for

absorption experiments in transmission mode.

Very stable beamline performance and smooth variation of the incident X-ray flux over 1 keV for EXAFS are necessary to detect weak spectral changes upon photoexcitations. In order to achieve pulse lengths that are by a factor of 10 shorter than the presently available 100 ps, considerable research and development by the machine group is necessary.

Estimated cost and staffing

The costs for setting up picosecond spectroscopy on ID26 are estimated as 800 k€ including a 10 kHz Ti:Sapphire LASER system and a fast chopper. In order to study very dilute systems or even low Z elements using the X-ray Raman technique, a very large-acceptance emission spectrometer is required. The cost for a spectrometer employing 40 analyser crystals is estimated to be 600 k€. The current performance of the monochromator on ID26 must be improved. A sub-standard white beam mirror needs to be replaced and a KB system has to be installed in front of the fast chopper for a cost of 600 k€. Total cost: 2 M€.

In order to realise this project while keeping up normal user operation, the ID26 staff requires support. The current beamline staff should be relieved from some of its duties by a beamline operation manager. An additional person should be shared between ID9 and ID26 for the operation of the femtosecond laser.

Existing or new BL/section/length/canted undulators

N/A

Timescale

In a first step, pump-and-probe experiments with nanosecond resolution can be achieved using a nanosecond laser (available from ID9), APDs and fast electronics. This could be realised beginning 2008. A picosecond setup with femtosecond laser could then be built by 2009/2010, depending on ID26 staffing.

Possible location

We propose to build a second experimental hutch at ID26 to host a laser system with emission spectrometer.

Computer/software needs

Automated data reduction and evaluation is necessary to deal with the large amount of data. The present project between ID26/ID24 and the Scientific Software Support should be intensified.

Detector needs

While a single APD suffices for a setup in back scattering (Bragg geometry), an array of up to 10 APDs could be used in Laue geometry.

Other needs concerning support groups, Associated Laboratories

N/A

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05: Nanoprobe energy dispersive XAS

Summary

We propose to add to the present ESRF capabilities a new[1] dispersive XAS nanoprobe beamline, working in the hard X-ray range (5-30 keV), optimised to perform XAS with ~ 300 nm spatial resolution. Dispersive optics allows for applications ranging from time-resolved studies at extreme conditions to 2D-mapping of heterogeneous samples, with full EXAFS information on each sub-micron pixel.

Scientific case

Non-uniform environments where the spatial inhomogeneity is of the order of a micrometer are ubiquitous in the three broad categories of earth/environmental, material/archeological and chemical/biological sciences. To date there have been very few tools to investigate such systems, none of which could be regarded as ideal. Sub-micron EXAFS, combined with fast acquisition, has the potential of providing previously unattainable insights into the structure and chemistry of a species, how these are related to its function and to that of other species that may coexist in complex systems, and how they evolve with time. In particular, besides the unique combination of spectroscopic and imaging capabilities, this instrument would open a unique door for *in situ* experiments. For example deep earth processes could be investigated by probing the chemistry of individual high-pressure phases typically less than 1 micron in diameter at equilibrium conditions in a complex chemical system such as that of the earth. At the other extreme of bacterial microbiology, an *in situ* X-ray nano-probe would give access to information at a single bacteria level in extreme conditions where cell metabolism involves metal based complex processes. Furthermore, bacteria in their media are very radiation sensitive systems. The possibility to record spectra very rapidly helps to identify and deal with radiation induced processes.

Technical aspects

MicroXAS beamlines worldwide (operational or planned) are all based on scanning XAS spectrometers. The most ambitious future beamlines aim for spot sizes of about 1 μm^2. The major challenge for these instruments will be to stabilise the focal spot position as a function of energy. In this context, a sub-micron spot size on a dispersive XAS beamline stands out as a very powerful alternative, featuring a rigorously stable focal spot, in both position and shape, and rapid acquisition. Experience on ID24 has shown that the present machine is able to improve steadily the stability of the electron beam. The proposed beamline offers a unique combination of a probe size of ~ 300 nm FWHM and rapid acquisition: ~1ms/eV for sequential acquisition of fluorescence and 10 ms/EXAFS spectrum for parallel acquisition of the transmitted intensity**.** Converted into 2D chemical imaging, this beamline will provide the unique capability of recording maps of 100x100 pixels in 100 s (transmission) and 2 hrs (fluorescence), with full EXAFS information in each pixel. This project will benefit from the synergy between 2 groups having unique expertise worldwide: in high brilliance dispersive XAS (ID24), and in sub-micron 2D-XAS techniques (ID22/ID21).

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[1] The present ID24 could be optimised for chemistry/catalysis (including industrial) requirements, that are, in general, not compatible with a small spot.

Estimated cost and staffing

The cost of this nano energy dispersive BL is estimated as ~5 M€.

We expect to welcome new user communities that are not familiar with EXAFS spectroscopy or imaging or both. These users will need constant help for acquisition and processing of the data. Furthermore, the processing of data (on-line and off-line) constitutes an essential aspect leading to the scientific success of the experiment, and also often requires the help of ESRF staff. This is why five staff members are required to run the beamline.

Existing or new BL/section/length/canted undulators

This new beamline requires one or more undulators on a high-ß section (allowing for shorter optics). The optical scheme could be compatible with the use of canted undulators (to be confirmed) on the ID24 straight section.

Timescale

Experience is being accumulated with the micro-XAS projects on ID24/ID22/ID21. The design of this new BL could start in 2008-2009.

Possible location

New location, or, if canted undulators can be envisaged, adaptation (or reconstruction) of a present beamline to allow the installation of this new BL on the same straight section.

Computer needs

As for other imaging techniques, the size of the recorded data is expected to be very large (Terabytes) and storage and processing of this data requires adapted memory and computing power.

Detector needs

Fast two-dimensional detectors exhibiting simultaneously a high dynamic range, high linearity and reduced readout time are crucial to achieve the scientific goal. Specific developments are required for fluorescence detection. Special attention will be given to normalisation detectors.

Other needs concerning support groups

One of the crucial points is the continuous work from the machine side for the stabilisation of the electron beam. Moreover, the estimated spot size for this beamline is totally dependent on the quality of the optics. Therefore, an important in-house R&D programme related to improvement of the optics (i.e. an IBF facility for large mirrors, better quality crystals) and metrology is mandatory. The present quality of the polychromator crystals is still below specifications for this future project. Finally, involvements of the sample environment laboratory for design and optimisation of specific sample environments compatible with a nanoprobe as well as that of a nanomanipulation laboratory for sample preparation will be required.

Associated laboratories

Several groups using the current spectromicroscopy capability of the ESRF would benefit from this new instrument. Active participation of groups in geochemistry, geophysics and archeometry can be easily anticipated.

06: Soft X-ray Beamline for High Resolution Resonant Inelastic Scattering and Photoemission

Summary

We propose a new soft X-ray beamline that would complement the existing soft X-ray facilities at the ESRF. The beamline would exploit resonant inelastic X-ray scattering and angle resolved photoemission in the 0.4 –1.6 keV range. Extremely small spots and very high energy resolution would open up new possibilities in studies of the electronic properties of materials and would utilise all the performance of the ESRF machine.

Scientific Case

Resonant inelastic X-ray scattering (RIXS) can be effectively used to measure the energy and symmetry of neutral electronic excitations in solids. In the soft X-ray range it is particularly useful for strongly correlated electron systems based on 3d transition metals and on rare-earths, because the excitation and de-excitation processes upon which RIXS is based directly involve 3d and 4f states respectively. As the RIXS final state is neutral and creates no core holes, the spectra are only limited by the intrinsic final state lifetime broadening and the instrumental energy resolution is usually the limiting factor for the detection of more and more detailed spectral features. The development of high resolution RIXS in the soft X-rays has been limited by intensity issues, due to the intrinsically small cross section of RIXS and by the small angular acceptance of spectrometers. At present only very few compounds have been measured with a combined resolution better than 1eV. In soft X-ray RIXS the best performances in terms of energy resolution are presently reached at ID08. The possibilities of high energy resolution are already interesting researchers not normally using X-rays.

Angle resolved photoemission (ARPES) has been an important tool in understanding the electronic structure of materials. Traditionally the work has been done in the VUV region where the cross-sections are large and high energy- and k-resolution are more easily achieved. In the last few years it has become clear that for certain studies the surface sensitivity of the VUV region is a problem. Typical examples are correlated materials, like rare-earth compounds or even the cuprates. Studies, for example at Spring8 and the ESRF (ID08), have shown that band structure information can still be obtained in the photon energy range 400-1500 eV with better bulk sensitivity but without reaching the XPS limit where only density of states information is achieved. In addition important information can be gained by utilising the absorption resonances in this energy region - 3d transition metals 400-1000eV and rare-earths 1000-1600eV. Having sufficient signal, high energy- and k-resolution in these energy regions, particularly up to 1600 eV, is a challenge for the future.

Technical Aspects

Resonant inelastic X-ray scattering and angle resolved photoemission are extremely demanding techniques because they require at the same time all the qualities of a modern X-ray beam line. For this project to succeed we need:

- Brilliance. The illuminated spot on the sample must be very small. The flux must be as high as possible because the cross section of the process is small.

State of the art focussing will be required.

- Resolving power. To perform a RIXS experiment with greater than 10000 combined resolving power the beam line monochromator must work at least at 20000 resolving power over the whole energy range. This is also exactly the type of resolving power needed for ARPES where the beamline is restricting the performance and not the analyser. Having energy resolutions of ten's of millivolts would be a great step forward.
- Stability. RIXS and ARPES experiments are intrinsically slow and long acquisitions are needed. The stability needs to be maintained when varying energy and polarisation. Future gains in the stability of the machine will be directly reflected in the data quality.
- Polarisation tuneability. The undulator source must be capable of delivering linearly and circularly polarised radiation with any orientation over the whole spectral range.

In addition we can further develop other aspects of the methods:

- Extended energy range. The 400- 1000 eV range covers all the $L_{2,3}$ absorption edges of 3*d* transition metals, light rare earth $M_{4,5}$ edges and oxygen and nitrogen K edges. High resolution RIXS and ARPES above 1 keV up to 1.6 keV would allow to cover all the rare earth $M_{4,5}$ edges. Such facilities would fully exploit the advantages of the ESRF in this energy range.
- Polarimetric RIXS measurements. Having the possibility of analysing the polarisation of the emitted photon would provide important additional information. Such measurements are extremely difficult in the soft x-ray range and a challenge for the future. At the higher energies crystal spectrometers could be employed that give easier access to polarisation analysis.
- Photon momentum transfer. The photon momentum is not negligible in the soft X-ray range and it can be advantageously used to complement ARPES in the exploration of band dispersion. In RIXS above 1 keV the maximum momentum transferred from the scattering photon to the solid is greater than 1$Å^{-1}$ meaning that the whole Brillouin zone of most lattices can be explored. Such measurements are difficult requiring the spectrometer to move about the sample but would provide essential new information.

The sum of all these requirements is *per se* a great challenge for any modern synchrotron radiation source. Moreover above 800 eV the ESRF, working at 6 GeV, has an intrinsic advantage over the other European synchrotrons (present and future).

Estimated cost and staffing

Based on previous projects we can estimate the cost at 5 M€. Staffing would need to be at the level of 5 staff.

Existing or new BL/Section/Length/Canted undulators

This beamline exploits the brilliance of the machine and needs to provide high flux, small spots and very high energy resolution. This would be best achieved on a dedicated beamline. The use of a canted undulator utilising part of an existing straight section might be possible.

Timescale

The design of this new BL could start in 2008.

Possible location

New location, or complete reconstruction of a present beamline.

07A: 30T steady magnetic fields for diffraction and spectroscopy

Summary

We propose to construct a beamline, with two end stations, dedicated to diffraction and spectroscopy experiments under steady magnetic fields up to 30 T. The Series Connected Hybrid magnets will share a common 10 MW power supply and cooling system. This power supply might also be shared by resistive magnet installations for neutron experiments at the ILL. Both stations will be complemented with very low temperature sample environments for studies of strongly correlated electron systems.

Scientific case

The magnetic field is a fundamental thermodynamic variable of importance equal to temperature or pressure. World wide there are many different laboratories dedicated to the production of high magnetic fields up to 45 T (steady fields), 80 T (pulsed, non-destructive), 120 T (pulsed, destructive), and 600 T (pulsed, destructive with flux compression). To date, however, X-ray and neutron experiments employ only superconducting magnets, which are intrinsically limited to fields below 17 T. A very large part of the phase diagram thus remains inaccessible to microscopic probes of magnetism.

Developments are under way in Japan and Europe to make pulsed magnetic fields available for X-ray and neutron experiments. Due to the low duty cycle (10 shots, i.e. about 40 msec of measurement time per hour), however, this technology is limited to experiments with very strong signals. Techniques that require very good statistics, such as XMCD, or that have intrinsically low count rates, such as inelastic neutron spectroscopy and resonant and non-resonant magnetic X-ray scattering, cannot be performed under these restrictions. This limitation is aggravated by the fact that many of the heavy fermion systems that undergo phase transitions of unknown nature in high magnetic fields have strongly quenched magnetic moments, and thus only very small magnetic scattering signals.

Technical aspects

The aim of this proposal is to make steady magnetic fields up to 30 T available to synchrotron X-ray and neutron experiments through the installation of a resistive magnet facility on the joint ESRF-ILL site. These two European large scale research facilities are among the world leaders in their respective domains of synchrotron x-ray and reactor-based neutron research. The main investment cost of such a facility is in the power and cooling infrastructure. The ESRF and the ILL offer the unique possibility to utilise the same power infrastructure at state-of-the-art X-ray and neutron facilities. This effectively halves the investment cost and further reduces the running costs, as compared to two independent steady field facilities.

The newly developed Series Connected Hybrid magnets of the NHMFL, Tallahassee, Florida, are the most efficient high field magnets available today: The operating power is reduced to 10 MW, as compared to 24 MW for a conventional Bitter magnet of equal field and sample volume.

Estimated cost and staffing

The investment costs are estimated as follows: 5 M€ for the X-ray installations, 13 M€ for a 10 MW power supply and the cooling infrastructure and 8 M€ per load magnet. Running costs include the usual beamline personnel (2 scientists and 2 postdocs) plus maintenance of the magnet systems (could be shared with ILL), and the price of electricity.

Existing or new BL/Section/Length/Canted undulators

We envision two end stations: One for diffraction with vertical field (3.5 – 100 keV), and one for spectroscopy (3.5 – 13 keV) with horizontal field direction along the beam axis. Both could be multiplexed of the same source device, as the power supply allows operation of only one load magnet at a time. The beamline could share a low-β straight section with canted undulators: The intensity of the incident beam has to be limited to avoid beam heating effects, which are common in very low temperature X-ray experiments.

Timescale

Due to its large scale, innovative technology and number of partners involved, this project requires a significant amount of planning before the construction phase.

Possible location

Safety considerations and the sheer size of the magnets require installation in a dedicated building outside of the ESRF main experimental hall. If the power supply is to be shared, a beamline oriented towards ILL is needed.

Computer needs

Standard

Detector needs

The detectors' sensitivity to stray magnetic fields must be addressed.

Other needs concerning support groups

Sample environment pool: A large percentage of the foreseen experiments will need very low temperatures, in the milli-Kelvin range.

Associated laboratories

It appears logical to undertake this project in collaboration with the ILL. We rely on the NHMFL for Series Connected Hybrid technology. A strong partnership with other European High Magnetic Field laboratories should be foreseen.

07B: Structural and Dynamical Properties of Matter at extreme P and T

Summary

The ID09A beamline is designed to determine structural properties of matter at high pressures in a diamond anvil cell (DAC) with the greatest accuracy possible by using monochromatic diffraction and large area imaging detectors. At present it is sharing a straight section and beam time with ID09B dedicated to ultra fast time-resolved diffraction.

We propose to extend ID09A to a fully dedicated high pressure diffraction beamline (on ID09 or elsewhere), including a detector upgrade for fast data collection with total elastic scattering capability and installation of a 1500 ton large volume press (LVP).

Scientific case

X-ray diffraction, which provides the structural information essential for understanding physical properties of matter, will remain the most widely used experimental technique to study crystalline, liquid, disordered or nanoscale materials under extreme pressures and temperatures.

ID09A and its offspring ID27 (formerly ID30) are major resources for the European physics, structural chemistry, material science and earth science communities. Both beamlines are in high demand and heavily oversubscribed. Extending ID09A to a fully dedicated beamline will increase the beamtime available for high pressure diffraction experiments from ~ 300 shifts to ~ 400 shifts per period.

ID09A is considered amongst the best DAC diffraction beam lines in the world with an intense development programme for improved sample environment like He-gas loading or cryostats for low temperature operation. The proposed detector upgrade combined with the high flux already available will allow new types of experiments. Real-time data collection during pressure and temperature increase will become possible. Mechanisms of pressure or temperature induced phase transitions can thus be studied. With a high dynamic range the total elastic scattering signal from the sample (Bragg reflections and diffuse scattering between the reflections) can be collected, to derive both structural and dynamic properties of matter under pressure.

Besides the earth science community, which presently uses facilities in Japan or the USA for experiments exceeding 15 GPa, the pressure limit of the Paris-Edinburgh (PE) cell, a LVP will also be interesting to the other user communities, e.g. to the materials science community for synthesising new (super hard) materials and in situ study of their formation. The structural properties of liquids, crystalline, disordered or nanoscale materials can be studied with very high resolution by measuring the total elastic scattering to very high Q-values.

Technical aspects

Photon fluxes on ID09A are high and exposure times are becoming quite short (< 10 sec for powder diffraction, less for single crystal diffraction). The bottleneck is the detector. The fastest online image plate reader (Mar345) needs 2 min for acquiring a single image. CCD-detectors with acquisition times of a few seconds are inadequate for work with DACs as they suffer from high background due to Compton scattering (from diamonds), strong signals (e.g. diamond reflections) combined with weak signals from the sample. Further to study weakly scattering materials, like molecular hydrogen at megabar pressure, the quality of the diffraction images has to be improved by the development of new detectors (see detector needs).

Further we suggest installing a 1500 ton LVP similar to the SPEED type used at Spring-8. The press should routinely reach pressures >40 GPa and 2500 K to cover earth's upper mantle and transition zone. Considerable effort should be made to increase the pressure range significantly by reducing the size of the (sintered diamond) anvils. Ultimately, pressures characteristic of lower mantle (90 GPa) should be reached to complement the measurements performed in a laser-heated DAC. Data should be collected with monochromatic radiation. Scattering from the sample container can be suppressed by a Soller slit system similar to the one already used for the PE cell. As detector we suggest a curved quasi 1-D pixel detector array with GaAs conversion layer, to work at high energies, high dynamic range and fast readout.

Estimated cost and staffing

Extension: 0.5M€, if ID09A stays in present location, else 2 M€. Detector: difficult to estimate (technology under development). LVP facility: 2 M€.

Additional to the present staff: one scientist, one postdoc and a technician. Further we suggest a technician for a LVP-laboratory.

Existing or new BL/Section/Length/Canted undulators

This beamline requires a low-ß section and an in-vacuum undulator for operation at high energies. Normal length with two experimental hutches (second hutch for large volume press). Canted undulators possible if the separation between the two branches is large enough for the experimental setup.

Timescale

Extension: as soon as funding becomes available. Detectors: technology under development, we estimate ~ 5 years until a working detector will exist. LVP: the planning phase (~ 1 year) can start immediately after a scientist has been hired; the building and testing phase will take about 2 years.

Possible location

Best: present location, hutches exist, minimum interruption of beamline operation, important because of high demand by user community.

Computer needs

As for other techniques using imaging detectors, the size of the recorded data is expected to increase over the current level to several Gigabytes/day and adapted storing capacity and calculation power is required. A strong effort has to be made on the software side. The large amount of data will make automated data processing and analysis indispensable.

Detector needs

We will need a new type of detector with the following characteristics: large area, high resolution (e.g. 50 x 50 cm with 5000 x 5000 pixels), as high dynamic range as possible, fast readout (10 ms), energy resolution for suppressing the background, no crosstalk between pixels. Pixel detectors are being developed to achieve this kind of performance. To work at high energies (> 30 keV) the detector needs a GaAs conversion layer.

Associated laboratories

Fully equipped laboratories for preparing DACs including gas loading system exist and are operated in collaboration with SES. Creation of a LVP laboratory with dedicated technician.

08: Long nanoprobe beamline and associated laboratories

Summary

We propose to add to the present ESRF capabilities a new 150 m long nanoprobe beamline, working in the hard X-ray range (6 – 50 keV), optimised to investigate spatial dimensions in the 50 nm range and below, with spots at the limit of X-ray focusing capability, devoted to imaging, spectromicroscopy and scattering. This beamline is complemented by a nano-characterisation platform and a centre for nano-optics devices.

Scientific case

Microtomography, micro-scattering, or spectro-microscopy, presently reach a spatial resolution in the 10^{-7} -10^{-6} m range. A gain of one order of magnitude (10^{-8} m scale) opens the very important area of nano-sciences, both for materials and biology. The proposed beamline aims to answer questions raised by modern science and techniques, and is intended to attract unique cutting-edge experiments in a broad range of disciplines, which include biology and medicine (role and chemistry of sub-cellular trace metal, cells, implants), soft condensed matter (scattering from single vesicles, fibre/matrix interfaces, hierarchical scales in biocomposites…) geochemistry (extreme conditions…), materials nanoscience (nanocrystals, electromigration, micro-structure, composition, plasticity …), Universe science (Mars mission, Stardust mission,…), environmental sciences (metals in plants, …) and cultural heritage. Fast experiments (in the ms to the few seconds range) are required to investigate evolving processes (functional follow up after injection of a drug in an animal model, liquid foams evolution, fracture propagation, phase transformation…): they are also within the scope of the proposed beamline.

Technical aspects

The techniques that will be developed include scattering from ultrasmall volumes and absorption, phase, or fluorescence, tomography on the nm scale. They offer unique capabilities (3D information, time-resolved, chemically selective). X-ray focusing limits are estimated to be in the 10 nm range. The present ESRF beamlines were not conceived to approach this limit. The proposed nanoprobe beamline should display the best coherence and focusing properties, and therefore be long (>150m). It will be based on the experience we already acquired on ID13, ID19 and ID22NI, but will be conceived from the very beginning to be optimized for nano-imaging and spectro-microscopy and ultra-small volume scattering using coherent beams. The 10 years experience of the ESRF in developing instruments with micron or sub-micron lateral resolution ensures that we can develop the knowledge necessary to perform the upcoming new nanoprobe technical requirements. This implies:

1) Technical developments both for the optics, sample environment and detectors to take into account the dose problem on biological samples as well as stable setups for the various techniques (interferometers for feedback and dynamic adjustment, and an improved stability of the X-ray source itself), “clean” elements (windows, monochromators, …) not reducing the coherence, and state of the art micro-focussing devices like CRL, FZP and KB multilayers
2) Pushing the energy resolution to combine the techniques (XANES tomography, for instance) and the detection limit of trace elements, presently in the ppm range, to reach the ppb one

3) Partnerships with other institutes, specialised in the fabrication of the needed optical/focusing devices.

Estimated cost and staffing

The cost of this nanoprobe beamline is estimated as 5 M€.

A substantial part of the users requiring nano-imaging or analysis know very little about SR and need a constant help for the acquisition and processing of the data. Furthermore, the processing of the data (on-line and off-line) constitutes an essential aspect leading to the scientific success of the experiment, and also often requires the help of ESRF staff. This is why five staff members are required to run the beamline.

Existing or new BL/Section/Length/Canted undulators

This beamline requires a low beta section, is long (~ 120 – 150 m) and will occupy a complete straight section

Timescale

Experience is being accumulated with the pilot project ID22NI. The design of this new BL could start in 2008.

Location

New location, or complete reconstruction of a present long beamline, moved to another location.

Computer needs

As for other imaging techniques, the size of the recorded data is expected to be very big (Terabytes) and the storage and processing of this data requires adapted computing power.

Detector needs

Two-dimensional detectors exhibiting simultaneously high spatial resolution (submicron range), high dynamic range, high efficiency and reduced readout time are crucial to achieve the scientific case. For scattering experiments, fast framing 2D detectors with single photon counting capability, high dynamic range and < 50 µm point spread function are required.

Other needs concerning support groups

The partnership with external institutes, specialised in the fabrication of optics/nanofocussing devices, implies the existence at the ESRF of a group active in these technologies.

Associated laboratories

A **nano-characterisation platform** with complementary instruments (electron, infrared, confocal microscopes, nano-manipulation, sample preparations etc,…) is needed. Its cost is in the 3 M€ range.

A **European Centre for the development and production of nano-optics devices,** resulting from a joint effort of the European synchrotron radiation community is strongly recommended since the success of this programme will rely on the availability of very high quality nano-optics devices. State-of-the-art devices are not commercially available in Europe. The ESRF location for such a centre is justified when considering the experience, skills and knowledge accumulated at the ESRF (and locally) on these topics. Its cost is at least in the 6 – 8 M€ range, and clearly requires European funding.

09: Long Pinhole Ultra Small Angle X-ray Scattering Beamline

Summary

We propose to add to the present ESRF capabilities a long (> 150 m) ultrasmall-angle scattering beamline, which will compliment existing USAXS/SAXS/WAXS capabilities. Science performed at this beamline would address large biological structures, higher scales in complex composite materials and transient processes in micron scale.

Scientific case

Small-angle X-ray scattering (SAXS) has emerged as a powerful method to elucidate the multilevel structure of nanomaterials. Thus the 10 m pinhole camera of the ID02 beamline allows resolving the fine structure in diffraction pattern from units with large repeat distances. For instance, the X-ray interference from a contracted muscle sarcomere turned out to be a sensitive technique to probe Å-scale motion of myosin molecules in the sub-millisecond time scale during active contraction. Many applications require, however, the higher Q-resolution of ultra small-angle X-ray scattering (USAXS), which is accessible until now only by the Bonse-Hart camera. Although these optics permits access to very low Q (< 10^{-3} nm^{-1}), it is a scanning method and therefore not suitable for studying transient processes (e.g. particle growth in an electrical arc) and most radiation sensitive biological and soft matter systems. In addition, data acquisition can be laborious, if not impractical, when investigating oriented samples. Therefore, it is highly desirable to have a long pinhole camera, which provides the Q-range, resolution and low background of the Bonse-Hart camera. This will initiate new applications of USAXS in biology and nanoscience and further exploitation of coherence in SAXS. Examples include structural elucidation of composite malignant biological specimen such as bones and tissues, crystallography of photonic materials, transient processes during nanomaterial growth, onset of polymer crystallisation, droplet fragmentation in sonic jets, etc. Most often, these applications require complex sample environments and complimentary SAXS/WAXS information. Therefore, it is important to retain USAXS, SAXS and WAXS techniques at the same beamline.

Technical aspects

The schematic layout for a long pinhole USAXS camera is shown below. A stable, virtual source is generated at 60 m from the source by 1:1 demagnifying optics. A second, 3:1 magnifying optical system demagnifies the source divergence by a factor of 3. This should allow a divergence of ≤10 µrad to be attained at the sample position. An on-axis focusing system based on a refractive lens with possibly a double-mirror system for harmonics suppression is persuasive but has to be compared with other focusing schemes in view of parasitic background suppression and stability of the long lever arm. For materials science applications it will be of interest to develop USAXS techniques for high energies (HUSAXS) and for anomalous scattering (AUSAXS). A further key requirement is the availability of a high dynamic range (24 bit) and high resolution (< 50 µm) large area detector (30 cm x 30 cm) with ideally millisecond time resolving capabilities. A photon counting detector is desirable but a low-noise, integrating detector might be sufficient for most applications.

Estimated cost and staffing

The staff of ID02 should be increased to 5 scientists in order to cope with the beamline extension. Estimated costs are 5 M€.

Existing or new BL/Section/Length/Canted undulators

New beamline; > 150 m long; high-beta section.

Timescale

Conceptual design and implementation could start once funding becomes available.

Possible location

The length of the beamline does not allow an extension of the ID02 beamline due to the obstruction by existing buildings external to the storage ring building. It is therefore proposed to reconstruct a combined SAXS/WAXS and USAXS beamline at a new location, which would also provide more space for annex laboratories.

Computer needs

The requirement for fast on-line reduction necessitates large data storage and processing capacity. In order to make the technique attractive to a broad scientific community, the modelling and simulation capabilities also need to be commensurate with the instrument characteristics.

Detector needs

A 2D detector with 24 bit dynamic range,< 50 µm resolution, 30 cm x 30 cm detecting area and with ideally millisecond time resolving capabilities is a prerequisite. This could possibly be a pixel detector if it can meet the above characteristics without dead detecting surface.

Associated laboratories

Laboratories for sample preparation (e.g. colloids), special sample environments (e.g. sonic jet, extruder, etc.), imaging (confocal microscope), mechanical probes (rheometer, tensile device, etc.), light scattering and optical tweezers. These laboratories could be part of the Soft Condensed Matter Partnership.

10: Time Resolved Diffraction

Summary

We propose to build a dedicated beamline for time resolved diffraction experiments covering the timescale from picoseconds to milliseconds applied to physical, chemical and biological systems. The undulators and the optics will be optimised for laser pump and X-ray probe experiments at energies between 15-30 keV. The beamline will have options for four-circle diffractometry on small molecules and time-resolved small-angle scattering.

Scientific case

The visualisation of atomic motions in physical, chemical and biological transformations is fundamental for the understanding of the relationship between structure and real-time interactions. In a transformation process, molecules (or atoms) typically pass though excited states with energy barriers that determine the lifetimes of intermediate structures along the reaction pathway. In many cases electrons, atoms or molecules can be activated by ultra short laser pulses that raise the energy above a reaction barrier. The ESRF has played a pioneering role in picosecond diffraction from proteins and in liquids. The aim of a dedicated beamline is to consolidate on-going efforts by having more time for commissioning tasks and in-house experiments that are very demanding. Secondly we propose to use the multibunch periods, that run about 68% of the time, for experiments on slower timescales, notably for millisecond and microsecond chemical crystallography and for time resolved small-angle scattering from biological molecules. Note finally that picosecond experiments at the ESRF are defining the way in which femtosecond experiments will be done on a future Free Electron X-ray Laser.

Technical aspects

A time resolved beamline needs a very intense undulator beam for short exposure times. Experience from crystal and liquid diffraction has shown that the best compromise between intensity, diffraction power, absorption and detection efficiency is 15 – 30 keV. Short-period in-vacuum undulators are ideal for this energy range and we propose to have two in-vacuum undulators with fundamental energies at 15 keV (U15) and 30 keV (U12). New advances in undulator technology with hybrid magnets and perhaps even cryo-magnets allow to increase the flux by a factor of 2 - 3 in the near future. We propose to upgrade the X-ray chopper to run faster, from 1.0 kHz to 1.2 kHz and have a 20 % larger rotor radius. The aim would be to increase the frequency of X-ray pulses on the sample to 3600 Hz using an ultra precise (triangular) rotor in the chopper. A heatload chopper producing 50 µs pulses of white beam, at the frequency of the experiments, should be installed after the primary slits.

An extensive laser facility next to the beamline is a key feature of this proposal. It is nowadays possible to increase the total power of a femtosecond laser from 1 W to 10 W. The laser should have an optical parametric amplifier (OPA) to shift the wavelength from the UV to the IR and provide set-ups for frequency doubling (400 nm), tripling (267 nm) and quadrupling (200 nm). We propose to install a four-circle diffractometer for small molecule diffraction and to equip the beamline with a 2.0 m long detector arm for SAXS.

Estimated cost and staffing

The cost of a new beamline including the laser facility is 6 M€. However if ID09 is dedicated to time resolved work, the price would be reduced to 1.5 M€.

The beamline should be staffed by two scientists, one beamline operation manager with laser experience, two postdocs, one technician, 1/2 mechanical engineer and 1/2 software engineer. This staff level is justified given the innovative nature of the experiments including the support needed to inexperienced users.

Existing or new BL/Section/length/Canted undulators

The beamline needs a low-beta section with a large experimental hutch stretching out to 60 m from the source point. The beamline seems incompatible with canted undulators due to the size of the optical elements including the heat load chopper in the optics hutch.

Timescale

If the high-pressure activities on ID09A are moved elsewhere, the upgrade could be finished within 18 months.

Possible Location

The obvious location is to stay on ID09 due to the large number of delicate components in the set-up. If this is not possible, the new location should have space for a large control hutch and a small chemistry lab. The beamline should be installed on a *low-beta* site to ensure a small 50-micron diameter focus from a toroidal mirror (M= 2/3).

Computer needs

The amount of CCD data is likely to increase by a factor of 10 due to the larger CCD detector and faster acquisition. Real-time data analysis will benefit from next generation processors at 5 GHz. The need for storage capacity will as well increase by a factor of 10.

Detector needs

A fast and large CCD detector is essential for the new beamline. We propose a MAR225 with its 1.5 s readout. The larger area will increase the resolution limit for smaller proteins, from 1.7 to 1.5 Å. A FReLoN detector should also be available for real-time acquisition on slower time scales. Beam diagnostics is essential for aligning the beams in space and in time and we foresee the use of small avalanche diodes and photo detectors coupled to high-frequency oscilloscopes (6 GHz).

Other needs concerning support groups

N/A

Associated laboratories

As described above.

11: "Micro/Nano-X-ray Diffraction": A new (canted) beamline branch at ID 13

Summary

We propose two independently operating branches for micro/nano-diffraction making use of canted undulators. The already existing ID13 Micro-Branch would aim for SAXS/WAXS experiments with a spot size of about 1 µm, a high flexibility in sample environments and automated data collection/data analysis features. The Nano-Branch should be optimised for nanodiffraction experiments with an emphasis on soft condensed matter and biological materials for beam sizes down to about 20 nm.

Scientific case

Wide-angle X-ray scattering (WAXS) and small-angle X-ray scattering (SAXS) experiments performed at the microfocus beamline (ID13) address a range of topics in soft condensed matter, biological materials but also in hard-condensed matter. Experimental techniques have been developed for single crystal diffraction and micro-SAXS/WAXS including grazing-incidence techniques (micro-GISAXS), which allows a positive cross-fertilisation. Thus the structures of amyloid micro-crystals as well as fibre orientation in single wood cells have been examined. R&D at the ID13 beamline has contributed to the conception of a number of microfocus beamlines worldwide.

Several X-ray optical systems have recently demonstrated the capability of reaching sub-50 nm focal X-ray beams at $E \geq 13$ keV. Refractive lens optics, commissioned by Schroer *et al.,* at ID13, is an example for this trend. Such optical systems will be implemented in the future ID13 Nano-Branch, which will be commissioned in 2007. The generation of coherent nanobeams down to about 20 nm focal spot size (e.g. by refractive lens optics) will provide new scientific opportunities such as the study of nanodeformed biocomposites or strained interfaces of semiconductor heterostructures.

The Nano- and already existing Micro-Branch of ID13 will not be operating independently as they will use the same undulator and monochromator. This implies that it will become impossible to develop all areas with equal intensity. A special effort will, however, be required for nanobeams, which will need completely new instrumentation and sample environments. Thus nano-GISAXS will allow studying gradient interfaces or the onset of protein crystallisation in nanolitre volumes. At the same time there is an increasing interest from new user communities with none or limited experience in synchrotron radiation instrumentation for SAXS/WAXS experiments with an about 1 µm diameter beam. Thus biologists might be interested in microfluidic *in situ* experiments of amyloid formation or *in vitro* studies of silk protein aggregation. Sample environments should therefore be very flexible and data analysis online. Scanning SAXS/WAXS should for example produce on-line composite images with local information on crystalline phase, SAXS-parameters etc.

Technical aspects

The two branches should be located at a canted undulator structure and would make use of the existing ID13 beamline as far as possible. Beams of both branches would be monochromatised in a common optical hutch, which would extend into the existing 1st experimental hutch of ID13. The undulator beam closer to the ring would pass through a channel-cut monochromator and from there on into the Nano-Branch hutch. The beam from the second undulator would be horizontally redirected by a double monochromator system and would then pass into the current second experimental hutch of ID13. All aspects of diffraction -including single crystal nano-diffraction, nano-SAXS/WAXS and nano-GISAXS/GIWAXS- would be developed in the Nano-Branch. The aim would be to investigate the smallest possible sample volumes. For organic and biological single crystal experiments this will require combining systematically sample rotation and translation in order to reach limits imposed by radiation damage. The Micro-Branch would specialise on beam sizes of about 1 µm by KB-mirrors for rapid scanning micro-SAXS/WAXS combined with automatic data analysis techniques. This branch would be flexible in terms of special sample environments such as deformation rigs or microfluidic cells. Complimentary techniques like micro-Raman or microfluorescence would be routinely available.

Estimated cost and staffing

The cost of installing two independent branches is estimated to amount to 3 M€, which covers the modification of the hutch structures, control cabins and the horizontally redirecting monochromator. This takes the ongoing refurbishment of ID13 into account. Both branches will have a close scientific collaboration and common technical staff.

Existing or new BL/Section/Length/Canted undulators

Both branches would be located at the ID13 beamline, which is currently installing a **Nano-Branch** with focusing optics at about 90 m from the source. The beamline will use canted undulators.

Timescale

The design of the modification and its implementation could start once funding becomes available.

Possible location

At ID13.

Computer needs

Scanning diffractometry using 2D detectors with on-line data analysis implies very big data volumes, which will require a local data processing cluster and local storage.

Detector needs

2D detector with – ideally - the following features: ms time resolution, single photon sensitivity, > 16 bit dynamic range, 30 x 30 cm^2 active area, $\leq$ 50 µm point spread function.

Other needs concerning support groups

Support for obtaining special optics including external collaborations

Associated laboratories

Microscopies: optical, SEM, AFM, nearfield; **sample manipulation**: FIB, laser dissection, laser tweezers, nanomanipulators; **microfluidics**; access to a future **Soft Condensed Matter Partnership** laboratory.

12: Scanning Hard X-ray photoelectron microscopy beamline

Summary

We propose to implement at the ESRF a new long (150 m) X-ray photoelelectron spectroscopy nanoprobe beamline, working in the X-ray range (= 1 - 25 keV), optimized for investigating by electron spectroscopy the chemical and electronic properties of bulk, interfaces, buried objects, and gas exposed surfaces with lateral dimensions down to the 50 nm range (and below), with depth information beyond 20 nm. Microscopy can be performed by scanning the sample with nm resolution. Photoelectron imaging and spin detection could be further options.

Scientific case

Scanning photoelectron microscopes at soft X-ray Synchrotron machines are already popular and fruitful instruments (e.g. BL 2.2.L at ELETTRA and BL 6.3.1 ALS). Spot sizes of around 100 nm are reached at ELETTRA together with an overall resolution of about 400 meV at around 500 eV photon energy. The probing depth is shallow, not exceeding about 2 nm. At hard X-ray energies and with sufficient energetic electrons, the energy resolution can be significantly improved and the probing depth considerably enhanced to beyond 20 nm. This is well documented in the proceedings[2] of the HaXPES workshop, which had been held at the ESRF in 2003. We envisage the following applications for the SHaXPES beamline:

- Material science: Scanning ESCA with better than 50 nm spatial and 100 meV to few eV electron energy resolution for analysis of the local chemical composition (nano-ESCA), e.g. for micro-electronic devices, grains and grain boundaries, clusters, dots, and domains in thin films, buried interfaces, etc.
- Physical Science/Solid State Physics: valence band and conduction band spectroscopy with about 20 meV to 500 meV energy resolution to determine local electronic properties of materials, devices, grains, grain boundaries and exotic crystals with spatial resolution down to 50 nm at depth exceeding 20 nm.
- X-ray photoelectron spectroscopy and chemical specification of interfaces reactions during gas exposure, e.g. for applications in catalysis. High electron kinetic energy and small sample size and suitable differential pumping would permit to investigate surfaces at gas pressures up to about 10 mbar).

Technical aspects

The key features of the beamline regarding the optical components are: (i) High flux, (ii) tuneability from about 2 to 25 keV, (iii) variable energy resolution from few eV down to about 10 meV, and (iv) a focal spot size down to 50 nm or better. This requires a long (about 150 m) beamline taking beam from a 5 m straight section with appropriate undulator(s), a primary monochromator and a high precision two-axis secondary monochromator. Because of the necessary energy tuneability, mirror focusing and KB, in-vacuum, close-focusing optics would be the primary choice. The HaXPES spectrometer, which is presently developed by the German company SPECS, will have to be further developed for the scanning microscope, especially adding/allowing suitable differential pumping stages for high (10 mbar) gas pressure

[2] Nuclear Instruments and Methods A, Volume 547, Issue 1, Pages 1-238 (21 July 2005) Proceedings of the Workshop on Hard X-ray Photoelectron Spectroscopy – HAXPES; Edited by Jörg Zegenhagen and Christof Kunz

work. A UHV compatible, ultra-precision, high resolution (5 nm) manipulator needs to be developed. A UHV (compatible) chamber with preparation (e.g., cleaving, sputtering, evaporation), diagnostic/alignment (e.g., microscopes) and analysis (e.g., AES, STM/AFM) tools is needed

Estimated Cost and staffing

The cost of building this beamline from scratch can be estimated as 5 M€. Standard ESRF staffing is estimated to be sufficient to operate the beamline. However, because of the complexity of the apparatus, short term contracted staff would be less efficient and either two permanent scientific staff or two second scientists would be needed.

Existing or new BL/Section/Length/Canted undulators

This beamline of 150 m length would be best placed at a low-ß section and will make use of the complete straight section.

Timescale

Experience is being accumulated with the HaXPES activities at ID32. A HaXPES spectrometer, which will allow detecting photoelectrons up to 15 keV with 20 meV energy resolution is currently being developed by the German company SPECS within the framework of a German BMBF project. This spectrometer is expected to be installed at ID32 in the beginning of 2007 and will allow gaining valuable information for the SHaXPES instrument. The design of the SHaXPES beamline could start in 2008.

Possible location

No suggestion for the moment.

Computer needs

Standard

Detector needs

The electron spectrometer for the SHaXPEM station needs to be developed by a commercial company. Work is already going on in that direction.

Other needs concerning support groups

Technical personnel with expertise in electron spectrometers and associated electronics should be integrated into, e.g., the BLISS group.

Associated laboratories

An off-line pre-characterisation laboratory providing XPS capabilities would be useful. Similar to the demand by other nano-focusing projects, nano-characterisation **facilities** with complementary instruments (electron, STM/AFM, infrared, confocal microscopes, nano-manipulation, deposition systems etc,…) are needed.

Additional Information

A SHaXPES instrument is presently developed at SPring8 by K. Kobayashi et al., utilizing electron optics to achieve sub-micrometer resolution. With this approach much intensity is wasted since the X-ray beam size is much larger than the spot of the electron analyser. However, the achievable spatial resolution can be higher than for the proposed instrument. It should be investigated if both approaches can be realized at the ESRF.

13: Engineering Materials Science beamline
Energy dispersive beamline for Engineering Materials Science

Summary

We propose to dedicate a bending magnet beamline to the field of engineering materials science in order to satisfy the increasing demand for the use of high energy X-rays in the range (20 - 100 keV). This BL operating at low maintenance and installation cost will be optimised for the energy dispersive diffraction technique using white synchrotron radiation from a bending magnet including as well a monochromatic operation for texture measurements. The key advantage of these techniques is that they provide high spatial resolution in large bulk samples. This beam line will release the increasing pressure on ID11, ID15, and ID31.

Scientific case

The engineering sector is a large potential user group for the ESRF and ILL facilities in Grenoble. However, ESRF and ILL have been constructed mainly with academic research in mind and the demands for applied engineering applications and academic research differ markedly. In 2001 the FaME38 support facility (Facility for Materials Engineering at ILL-ESRF) was created through a start-up grant from EPSRC with matching support from the ESRF and ILL to facilitate the engineering use and to provide information and advice for engineers with little or no experience in the use of these facilities. The initial phase of this project ended in 2005. The project was evaluated by an external panel of experts which concluded that the initial phase was successful and the panel recommended that the project should be continued. The continuation is now under way and an initial grant from the ESPSRC has been approved. The initial objectives for the start up phase was:

1) To provide a joint support facility at the ERSF-ILL to encourage and to facilitate engineering research
2) To provide a technical centre with standard mounting facilities and auxiliary equipment such as stress rigs etc
3) To provide a Knowledge and Training Centre
4) To provide a “Location” for visiting engineers
5) To provide engineering expertise to the ESRF/ILL
6) To encourage routine engineering research
7) To facilitate commercial exploitation of the instruments

The initial phase of the project has been successful and the use of the ESRF by engineers, notably from the aeronautics and energy industry, has markedly increased and will further expand when industrial standards are properly established. The experimental work has mainly been concentrated on beamlines ID11, ID15, ID31 and ID19 for stress/strain and imaging applications. All of these beamlines are heavily oversubscribed since they are the flagships of Materials Science research at the ESRF. It has been realised that some of the engineering applications do not need the ultimate performance of insertion devices but rather the rapid access to dedicated set-ups for stress/strain and imaging/tomography. The implementation of a dedicated bending magnet station for engineering applications for light materials would thus both provide a tailor made facility for engineering research and alleviate some of the demand on the present insertion device beamlines.

Technical aspects

A bending magnet beamline will provide useful X-rays below 100 keV and allow assessing mainly light materials like Al and Ti alloys typically used in the aerospace manufacturing sector.

To a large extent such a beamline can be operated in an "automatic mode" since the experimental setup is fairly standardised. It uses only the white beam and an energy dispersive diffraction technique requiring slit systems and Germanium solid state detectors at a fixed 2? angle. For texture studies an easy to operate fixed exit bend Laue monochromator (similar to the ID15 model) combined with a 2D detector can be added.

Tomographic and other imaging techniques are envisaged in combination with diffraction techniques.

The manipulation of heavy and large components has to be foreseen.

Such a dedicated beamline with an optimised, fixed setup allows reducing the experimental setup time leading to a more effective use of beamtime. Analysis software already exits (FaME38; based on GSAS, Los Alamos National Laboratory) which allows the near-online data reduction and can be further developed (automated alignment, calibration, efficiency,…). The main aspects are the gain in reliability and the repeatability of measurements with high spatial resolution in bulk samples. These are unremitting conditions to increase the trust in the technique in order to attract industrial customers.

Estimated cost and staffing

The cost of this Engineering Materials Science BL can be estimated to 5.0 M€.

This new beamline can be integrated to the present ID15 operation as 2nd half of ID15B: 1 scientist, 1 postdoc. Furthermore the FaME38 staff will be used for beamline operations.

It can be considered as a low maintenance beamline which would be close to automatic functioning: the general technical support can be guaranteed by existing technical personal. The routine operation of stress rigs will require training of the technical personal.

Existing or new BL/Section/length/wiggler

This beamline will be installed on a bending magnet. Ideally a wiggler site would be used.

Timescale

Experience about the engineering needs for projects like this has been accumulated during the present operation of the ESRF Materials Science beamlines. The design of this new beamline could start once funding becomes available and it could be operational within less than 12 months depending on availability of technical service and delivery of material.

Possible location

Upgrade of a present bending magnet beamline. If any of the present operating bending magnet stations would become available the time and cost requirements would be reduced and a location close to ID15 would be advantageous for operational reasons.

Computer needs

Today's standard requirements (control, online data analysis for in situ studies).

To facilitate on-line analysis and tomographic and other imaging techniques considerable computing power is needed. In particular the storage capability would be in the Terabyte range.

Detector needs

The energy dispersive technique would require 2 (+ 1 spare) Germanium solid state detectors and digital data processing electronics as basic setup. Texture measurements would require a standard 2D-detector as available today and the ongoing development of pixel and amorphous silicon/selenium detectors would be of large interest. The lower flux from a bending magnet station could be compensated in part by a larger number of germanium solid state detectors.

Other needs concerning support groups

Engineering specific sample environment: maintenance and operation of stress rigs by an existing technician.

Development of data analysis strategies and software for “automatic operation” (computing support).

Associated laboratories

At present the FaME38 laboratories at ILL are available for offline preparation of experiments.

Collaboration with research centers focused on engineering material science (FaMe38: consortium of UK universities; MPI for Iron research, Germany; TU Berlin).

Coordination Center for Engineering Materials Science (new national sources benefit from the technical and methodical development pushed at the ESRF).

14: A Coherent Diffraction Imaging Facility

Summary

We propose to split ID29 using canted undulators, one undulator providing an automated phasing facility specialised in the use of microcrystals. The other facility would provide a facility for the use of coherent diffraction imaging from biological samples to a spatial resolution of ultimately 20 nm.

Scientific case

The investigation of the large scale structure of cellular life and cellular machinery is generally studied by electron microscopy. For cellular imaging thin slices of the cells are required because of the limited penetration depth of the electrons. For the imaging of macromolecular assemblies the greatest success is limited to highly symmetrical systems in particular icsohedral viruses. In recent years there has been considerable interest in coherent diffractive imaging on noncrystalline specimens using coherent synchrotron radiation. This technique has the dual advantages of increased penetration depth so that intact cellular system may be imaged, and the capacity to reconstruct non periodic objects. Recent results (Shapiro *et*-al & Sayre PNAS, 102, 43 15343) have demonstrated that the spatial resolution available complements that of the best electron microscopy. Our aim will be to develop a facilty capable of achieving spatial resolutions of 20 nm from biological samples. At this resolution we would be able to identify components within a cell, and place the components (structures elucidated by MX) within macromolecular assemblies.

Development of a coherent diffraction imaging beamline for biology represents a considerable opportunity for the ESRF, potentially opening new avenues of research for biological systems and would span a resolution gap that exists between the study of biological systems (ID17) and the atomic resolution achievable with macromolecular crystallographic techniques.

Technical aspects

By installing canted undulators on ID29 we expect to maintain the excellent performance of the MX facility with further emphasis on the evolution of MX on micro-crystals.

In order to build a coherent diffraction imaging facility we expect to operate at energies between 3 and 7 keV. With a 60m long beamline we expect a coherent beam size of 50(H) µm × 300(V) µm in the unfocused beam, and 1 µm x 1 µm in the focused beam.

A significant radiation damage problem exists for biological samples and research must be initiated to develop tolerable methods for mitigating the effects.

Estimated Cost and staffing

Basic redevelopment with canted undulators 3.5 MEUR.

Staffing: ID29 would become two interacting beamlines with different staff complements. With careful matching of requirements for the two beamlines it should be possible to operate with staff equivalent to 1.5 ESRF beamlines.

Section/Length/Canted undulators

ID29 with canted undulators provides an appropriate source.

Timescale

Construction of the coherent diffraction imaging beamline would need an extended experimental hall. Background work needs to begin in the near future to allow sufficient time for the preparatory work to be undertaken.

Possible Location

ID29

Computer needs

Many Terabytes of data storage, maintained to allow secure (remote) access. Compute clusters to allow the most efficient data treatment. GRID based to allow for effective collaboration with the groups responsible for the samples under examination.

Detector needs

For the macromolecular diffraction part suitable systems are expected to be available. Coherent diffraction imaging needs investment in suitable detectors (large aperture, small pixel, photon counting)

Other needs concerning support groups

Development of this facility will have broad complementarity to activities in other areas at the ESRF and with the PSB/IVMS. Greatest success is ensured if the correct collaborations are established at the earliest opportunity.

Associated Laboratories

The Partnership for Structural Biology forms an ideal base

15: Massively Automated Sample Screening Integrated Facility

Summary

We propose to split ID14 using canted undulators, one undulator providing an automated phasing facility, the other providing a set of linked MX data collection platforms to provide a massively automated facility for the screening of diffraction quality samples.

Scientific case

As the complexity of biological problems under investigation continues to increase, the difficulty of obtaining high quality diffraction from these samples rises considerably. Even once crystallisation is achieved, structure determination is by no means straightforward. We propose to address this issue at the ESRF by the delivery of a Massively Automated Sample Screening Integrated Facility (MASSIF) for MX designed to deliver the maximal production of high quality MX data from problematic samples.

Investigation of the most complex problems will require screening very large numbers of crystals in order to obtain the best possible crystallographic data. It will become routine to need to screen, record and compare hundreds of samples before a complete and useful data collection set can be acquired.

Such a system would be equally attractive to the screening demand of the pharmaceutical industry. In addition, access to complementary techniques on the same beamline complex will allow complementary structural information to be obtained.

Technical aspects

With the experience of the canted undulator system of ID23, ID14 could be redeveloped as a beamline using a similar system. Using one of the canted undulators, ID14-4 would be tunable over the range 5 to 25 keV (compared to the current energy limits of 10.0 keV to 13.5 keV imposed by the ID14 side-station geometry). The second canted undulator would act as the radiation source for a series of fixed-energy side-stations employing thin transparent diamond monochromators. By radically modifying the optical design, the side stations will gain in stability and intensity. There would exist the possibility to build at least three side stations and potentially up to six.

Further flexibility could be introduced by the use of micro-stations for the fixed energy beamlines. More experimental stations could be fitted into the space with additional diamond monochromators ranged in the optics hutch. Many beamlines would mean a gradual reduction in intensity (a reduction in beam intensity of 4.3%/100µm of diamond at 12.7keV or around 6.5% per diamond monochromator using 100µm thick diamonds with an asymmetric Laue cut as currently on ID14). Many applications, such as initial sample screening, SAXS on protein solutions or a test-bed (to allow dedicated off-user testing of new instrumentation and software developments) would not require a particularly intense X-ray beam. Our proposal may thus prove an efficient way to enable many complementary techniques to be brought together on one undulator source.

The construction of more than three side-stations would open further possibilities, for example an open plan hutch containing several goniometers and a sample "shunting-yard" to pass samples automatically from a central storage area to multiple sample changers with appropriate resources. This facility would then become the core of MASSIF.

Estimated cost and staffing
Basic redevelopment with canted undulators: 3.5 M€.
With MASSIF: 4. to 4.5 M€

Manpower required to operate such a facility would be dictated by the degree of automation. It would be appropriate to consider the training and employment of "beamline operators" who would run the most highly automated facility.

Existing or new BL/Section/Length/canted undulators
ID14 with canted undulators provides an appropriate source.

Timescale
Phased closing of ID14 would need to planned in consideration with other MX beamline operations. Intial reconstruction would take 18 months to 2 years. Deployment of MASSiF: additional 24 months.

Possible location
ID14

Computer needs
Many Terabytes of data storage, maintained to allow secure (remote) access. Compute clusters to allow the most efficient data treatment. GRID based to allow for effective collaboration with the groups responsible for the samples under examination.

Detector needs
For MASSIF the largest CCD detectors are not necessary. However the tunable beamline would benefit from the largest, most sensitive detectors available.

Other needs concerning support groups
MASSIF implies that highly reliable and automated sample environments will be available – significant input is expected from existing Support Groups and Services.

Associated Laboratories
The Partnership for Structural Biology forms an ideal base

16: A bending magnet "Small-angle X-ray Scattering" beamline dedicated to functional biology and applied soft condensed matter research

Summary

We propose to add to the present ESRF capabilities a bending magnet small-angle X-ray scattering beamline for protein solution scattering and applied soft condensed matter science. The beamline will provide rapid screening capabilities for biological solution structures in the context of the Partnership for Structural Biology (PSB) and the macromolecular diffraction programme. It will also allow high throughput SAXS/WAXS experiments for applied soft condensed matter science including industrial applications. The beamline would provide turnkey-style operation with highly automated data processing capabilities.

Scientific case

Small-angle X-ray scattering (SAXS) provides low-resolution structural data of large proteins or biological complexes in solution. Routine use of this technique has become possible due to freely available data analysis software developed by Svergun et al. in recent years. The possibility of screening a large number of proteins in solution can provide invaluable information for guiding efforts in protein crystallization. One of the aims of the FP6 *SAXIER* design study project (involving the major European synchrotron radiation SAXS-beamlines including ESRF) is automating data analysis to a level that could, for example, be combined with protein separation by a chromatographic column. A bending magnet SAXS beamline is therefore of considerable interest for functional biology applications in the context of the PSB and macromolecular crystallography efforts.

Applied soft condensed matter (including industrial research on colloids, rheology and polymer crystallization) is a further target for a SAXS/WAXS bending magnet beamline. Experiments in this area often do not require the high brilliance of an undulator SAXS/WAXS beamline but the rapid throughput of a turnkey-style operating beamline. Experimental techniques and scientific applications developed would, however, facilitate their introduction at undulator beamlines of the soft condensed matter group (ID02/ID13 ...). Given the current interest in genomic research it is arguable that the share of protein solution scattering should be at least 50% of the total beamtime.

Technical aspects

The beamline could be equipped with a channel-cut monochromator and a complimentary double-multilayer monochromator for the highest stability and highest spectral brightness. Focusing could be based on mirror optics, refractive lens optics or a combination of both providing the highest possible stability and the lowest background. In view of low background requirements, a 2D gas-filled detector is proposed for SAXS and a 1D gas-filled detector for WAXS. A pixel detector is a future option.

A particular effort will be required for providing user-friendly beamline operation and automated data reduction/data analysis possibilities. Note that SAXS solution

scattering software tools developed in the context of the FP6 SAXIER project aim for an on-line construction of structural models from the SAXS data.
Applied soft condensed matter will in particular require adequate neighbouring laboratory space for the development and testing of special sample environments such as extrusion devices or rheometers.

Estimated cost and staffing

Estimated cost is 2 M€. Staff should comprise 2 scientists, 2 postdocs and a technician.

Existing or new BL/Section/Length/Canted undulators

New bending magnet beamline.

Timescale

Conceptual design and implementation could start at any time.

Possible Location

The beamline should be ideally located next to an undulator SAXS/WAXS beamline.

Computer needs

Online data reduction capabilities.

Detector needs

A 2D gasfilled detector for SAXS and a 1D gas-filled detector for WAXS. In the future, a pixel detector could be used in case the active surface could be large enough.

Associated Laboratories

Laboratories related to the PSB, macromolecular crystallography and the soft condensed matter group. A laboratory for testing of special sample environments (e.g. extrusion set-up, rheometer) should be close to the beamline.