

UPBL7: Soft X-rays for magnetic and electronic spectroscopy	
Current designated sector:	Facility goes to:
ID08	ID08

1.1 SUMMARY

The beamline will provide new facilities for the user community using soft X-rays at the ESRF to study the electronic and magnetic properties of materials. The aim is to strengthen and maintain a world leading position in this field by focussing on studies using dichroism and resonant inelastic X-ray scattering techniques. By building on 15 years of experience, we will provide a state-of-the art facility for absorption spectroscopy (with sophisticated sample environments and tuneable X-ray beam sizes from microns to 100's microns). In addition, an instrument with unprecedented high energy resolution for Resonant Inelastic X-ray Scattering (RIXS) will be built, again incorporating sophisticated sample environments. The facility for X-ray absorption will meet the demands of the very large and expanding user community using magnetic dichroism techniques and soft X-ray inelastic X-ray scattering has the potential to bring a new complementary tool for scientists who traditionally have used other methods like optical techniques, inelastic neutrons, electron energy loss etc.

1.2 PROJECT HISTORY

The UPBL7 project evolved from reflections on the ESRF long term strategy as outlined in the "Purple Book" (See sections 1.4 p72 and also 1.1 p16).

In October 2007, the ESRF hosted a special users meeting to discuss the Upgrade Programme with external experts reporting on the various areas of research. As a result of that meeting and following the advice given, a much more ambitious soft X-ray project was proposed which aimed at very high energy resolution for Resonant Inelastic X-ray Scattering and small beams for both RIXS and X-ray Absorption Spectroscopy. To enable this project and also to allow in the future for the possible use of very high magnetic fields (see section 2.4 of the Purple Book and in particular 2.4.5 p133) a long beam line (120 m) was envisaged.

In October 2008 a brainstorming was held to obtain the input of users and external experts on this project. The aims of the UPBL7 project were strongly endorsed.

1.3 SCIENTIFIC CASE

Historical background

The original ESRF soft X-ray beamline was ID12B, which was a branch line on ID12. Both the hard X-ray (ID12A) and the soft X-ray (ID12B) branches could work in parallel using canted undulators. As ID12B could be operated separately it became an independent beamline with its own staff in 1994. It started operation with users in March 1995. In November 1998 the beamline was reviewed for the first time. As a result a dedicated straight section for soft X-rays was allocated on ID08 and the beamline moved from ID12 in December 2000. User operation restarted on ID08 in February 2001. The beamline was further reviewed in May 2007. The committee recommended that to maximise future impact, the work at ID08 should focus on X-ray magnetic circular dichroism (XMCD), resonant X-ray inelastic scattering (RIXS) and soft X-ray angle- and spin-resolved photoemission. They also recommended upgrades including a new high-field magnet for XMCD and improvements to the X-ray spectrometer for RIXS. Also the assessment of the possibility of two branchlines, or in the longer term, two distinct beamlines for soft X-ray research was recommended.

Motivation for the upgrade

ID12B/ID08 was the first soft X-ray beamline on an insertion device giving full control of the polarisation (linear and circular). As the reviews of the beamline have shown, the beamline is highly competitive worldwide and there has been a strong push for more soft X-ray facilities at the ESRF for many years. The growth of national facilities has now helped to increase the possibilities for users elsewhere but, nevertheless, the ESRF facilities continue to be heavily oversubscribed. The Upgrade Programme gives the possibilities to move forwards with the experimental facilities that the ESRF can offer in this domain and will also allow it remain at the forefront worldwide. Through the process of developing the Long Term Strategy and taking into account the recommendations of the beamline reviews, the project has focussed on two main areas: very high energy resolution resonant inelastic X-ray scattering and X-ray magnetic circular dichroism. We believe that these developments will provide unique experimental facilities for absorption spectroscopy and in addition open new possibilities for inelastic X-ray scattering.

It should be noted that the possibility of small spots and a large space for sophisticated experimental end-stations is only made possible by the long beamline and the new building extension.

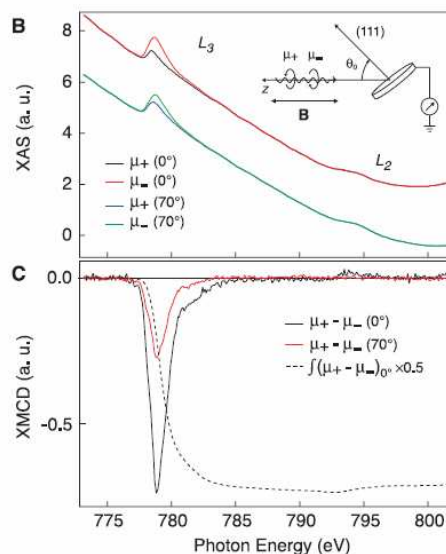
Science driving the beamline development

The current ESRF soft X-ray beamline (ID08) works in the broad scientific area of “magnetic and electronic properties of matter”. The new beamline, that would replace it, would still concentrate on science in this domain but would focus on providing specific advanced scientific tools to keep the soft X-ray activities at the ESRF at the forefront of research. The new possibilities presented by the UPBL7 project would allow investigations to be undertaken which are not possible today. It should also be noted that although the science that can be done is often of fundamental nature, many of the objectives have direct implications on applications, e.g. in spintronics.

One of the principle research areas identified was the study of magnetism and electronic structure of strongly correlated materials and, in particular, studies of spin, orbital and charge degrees of freedom in these materials. A main area is the study of 3d transition metal oxides, such as the titanates (Ulrich et al, 2008), vanadates (Braicovich et al, 2007), cuprates (Ghiringhelli et al, 2004) or multiferroic materials where the interplay of electrical and magnetic properties is of great interest. Other related scientific areas are the studies of heavy Fermion materials - for example studies of magnetic critical phenomena - and frustrated magnets. Momentum dependent studies with very high energy resolution will allow access to novel, fundamental excitations many of which cannot be studied easily today. Examples are orbitons, bi-magnons (Braicovich et al, 2009), phonons etc. Such studies will be of great interest to a wide scientific community outside the present X-ray user groups, e.g. coming from optical spectroscopy, neutron scattering, electron spectroscopy, and will also be of relevance to current theoretical efforts worldwide.

Another clear area is the study of low dimensional systems (e.g. Gambardella, 2007) - “few atom systems” - here the relationship between dimensionality and magnetism is of basic interest whilst the study of nanomagnets and nanomaterials, in general, is both of fundamental and applied relevance when one considers spintronic applications. Dynamical studies of such nano-objects are a major challenge. Other areas that can be well addressed by these techniques are dilute magnetic semiconductors (e.g. K. W. Edmonds et al, 2004, Y. Takeda et al, 2008) - here the elemental and high sensitivity of the soft X-ray techniques is vital.

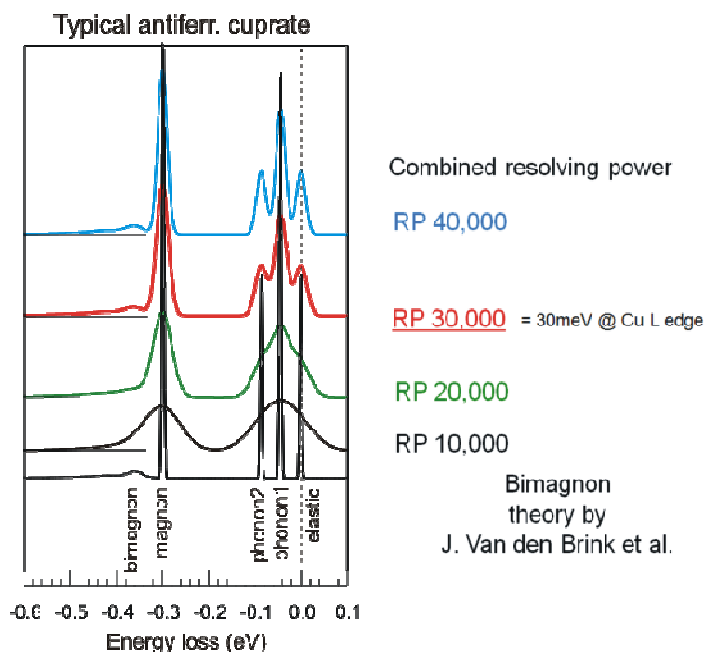
Along similar lines but not necessarily in the “nano-world” are studies of “new” or “tailored” materials. For example, multilayers of metals or compounds (e.g. oxides, Salluzzo 2009), which show different properties from their individual components are of great interest and a case where other techniques often do not have the sensitivity. The figure on the right shows the XMCD signal from 1% of a monolayer (ML) of cobalt on a Pt surface (Gambardella 2003). The sensitivity today is $<0.002\text{ML}$. In addition, the chemical, orbital and magnetic selectivity of the X-ray techniques is also of paramount importance. Other examples of scientific areas of interest are the study of molecular magnets - e.g. Gambardella et al, 2009 and Mannini et al, 2009 - (light elements like oxygen and nitrogen can also be studied), biomagnets and hard magnetic materials - here the elemental sensitivity to both transition metals and rare-earths is a great advantage. In materials science one could also think of using the new small spot capability to do combinational studies.



It was also made clear that the proposed beamline could be a very important instrument in the study of liquids (e.g. aqueous solutions (Fuchs et al, 2008)) and gases. Special cells, with ultra-thin windows, allow studies of liquids, gases and liquid/gas interfaces even when the rest of the instrument is under UHV vacuum.

Scientific capabilities that are at present not accessible at the ESRF

Resonant inelastic scattering will become possible with an energy resolution much higher (>30000 resolving power) than today. The figure shows an example of the gain in information that high resolution gives for the case of the cuprates. With a combined resolving power of 30000 or higher, features are resolved and line shapes can be determined that are not possible with poor resolution. Specialised sample environments could allow studies as a function of temperature (down to low temperatures, $\leq 4\text{K}$) and magnetic field, further expanding the scientific capabilities.



Complete magnetic dichroism (both circular and linear at the same time) measurements would become possible with a UHV vectorial high field magnet. Improved sample manipulation and lower sample temperatures ($\leq 4\text{K}$) will expand the range of materials that can be studied (e.g. small samples, low temperature phases of correlated materials, molecular magnets etc). Space for sophisticated sample preparation (e.g. in situ UHV surface science methods, pulsed laser deposition etc) and characterisation tools would enhance the scientific possibilities. Many of these methods would take advantage of the UHV environment inherent to the beamline and its experimental stations. Variable sized beams from 100's microns to the micron will allow many different samples to be studied, from those that need low photon density to avoid damaging, to very small crystals. Moreover, small beams would open the possibility of magnetic characterisation of combinational-type sample libraries of novel magnetic materials. Pushing to smaller length scales, maybe using local probes, could allow single nano-objects to be studied individually.

Possible future (mid- to long-term) developments after this beamline has become operational

The prospects of the very high DC magnetic fields ($>30\text{ T}$) should be seen as a medium or longer term development. Such an endeavor would have to be part of a partnership to be realistic. The new beamline being part of the "Magnetism Village" was seen as an added bonus in this respect.

Further the possibilities of improving the combined resolving power for RIXS experiments beyond the initial goal of 30000 was thought to be something to take into account from the beginning. This could be exploited when advancements, for example in detectors, allow them.

Also the further reduction in beam sizes (<1 micron) for future applications was thought to be desirable for some experiments but possibly for the longer-term. In this respect the combination of X-rays with local probes (e.g. STM (Eguchi, 2006)) should be considered.

There was also a feeling that, whilst the beamline should be optimised for the two main scientific objectives (inelastic scattering and dichroism studies), space for further developments should be allowed for in the design. The available floor space in the new building is well suited for this strategy. One possibility in this respect would be the extension of X-ray detected ferromagnetic resonance experiments that are being developed on ID12 (Goulon et al, 2005/2006), and elsewhere (Boero et al, 2005), on the future beamline. There would also be space for other activities that are currently carried out at ID08 including magnetic X-ray scattering (in particular coherent scattering), photoelectron spectroscopy, XPEEM microscopy etc.

1.4 TECHNICAL CONSIDERATIONS

X-ray source

Location: The new beamline would replace the existing ID08 beamline and take advantage of the existing infrastructure within the experimental hall. The new experimental facilities would be located in the extension building. This is consistent with the SAC approved floor plan and means the beamline could be on the floor as soon as the new building can be occupied.

Front end: As is the case today, a windowless UHV front-end is required. Special care needs to be taken to prevent the power generated in the vertical plane by the exotic undulator to heat chambers in the front-end. This is a known problem and solved on ID08. The power will be increased by approximately a factor of three due to the increase in the number of undulators and ring current.

Undulators: For a 6 m straight section an additional APPLEII undulator of ~2.5 m would be added (under study by Insertion Device Group). This would complement the existing two 1.6 m undulators and have the same period to give an effective length of 5.7 m. In the future with a 7 m straight section one can envisage having two 2.5 m devices and a 1.6 m device (6.6 m). The new devices would have the same period (88 mm) and field (0.62 T/0.56 T) and give linear (horizontal and vertical) and left/right circular polarised light. Since we will only work at the first harmonic the polarisation rate will always be close to 100%. The new device would give us the additional flexibility of rotating the linear polarisation vector continuously from +90 to -90 degrees (presently 0-90 degrees is possible). The gain in flux is ~3.5 compared to today. This is shown in the table below where the flux is calculated using the SRW programme.

APPLEII	300mA @ 400(1900eV) Circular
5m = 1.6m + 1.6m (today)	1.4 (0.9) x 10 ¹⁵ ph/sec/0.1%BW/200mA
6m = 1.6m + 1.6m + 2.5m	4(2.4) x 10 ¹⁵ ph/sec/0.1%BW
7m = 1.6m + 2.5m + 2.5m	5(3) x 10 ¹⁵ ph/sec/0.1%BW

Schedule for insertion devices:

A new 2.5 m could be used today on ID08 (replacing a 1.6m device) and should be put into the design phase as soon as possible. With the availability of the 6 m straight section the two 1.6 m devices can be used and if a 7 m section is developed a second 2.5 m device would need to be constructed.

General comments on the source:

The new beamline will use all modes of the machine and benefit from 300 mA current. Flux hungry experiments like the RIXS will mostly benefit from full current multibunch modes (50%). Stability is very important and any improvement compared to today will benefit both RIXS and absorption experiments (critical in this case). Stability over timescales from hours to milliseconds is important for the range of experiments envisaged. The use of 16 bunch for experiments using time-of-flight detectors is envisaged but is not the main thrust of the new beamline. The use of top-up could benefit fixed energy experiments but might complicate scanning experiments.

Bremsstrahlung shielding:

Since the beamline works in the soft X-ray range, typically <2 keV, the need for lead hutches is not mandatory for the entire beamline. This is the existing situation for ID08. On the new beamline it is proposed to use a double mirror as the first optical device. This would offset the beam by ~20 mm if we follow the ID08 scheme. This device is housed in the lead hutch. After this device we use a Bremsstrahlung stop which stops the on-axis radiation but allows a beam of X-rays to pass ~20 mm off axis. On ID08 there is also a vertically deflecting mirror before the final lead back wall of the hutch. In the present optical scheme for the new beamline this mirror would not be present.

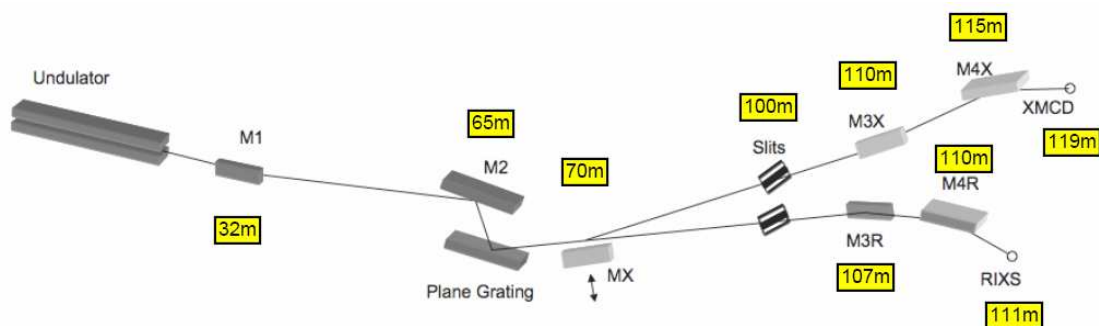
Beamline requirements:

The beamline should be designed for principally two types of experiments:

1. Resonant inelastic X-ray scattering that requires very high resolving power ($\geq 5 \times 10^4$) and a micron spot size in the vertical (dispersion) direction - this will be optically matched to an analysing spectrometer also providing the same resolving power to give an overall ~30000 resolving power - and
2. X-ray dichroism that requires moderate energy resolution ($\sim 5 \times 10^3$) over a range of approximately 100 eV when scanned at 1 eV/s as well as a variable spot size (micron to 100's microns). Both techniques require good energy reproducibility, low harmonic contamination, highest possible flux and stability in energy and position. Since the spectrometers and end-stations require significant space, the beamline should extend into the new building and provide sufficient space around the sample whilst also achieving small spots. The beamline energy range should be optimised over the energy range of 300 to 1500 eV but extends to at least 2000 eV.

General layout:

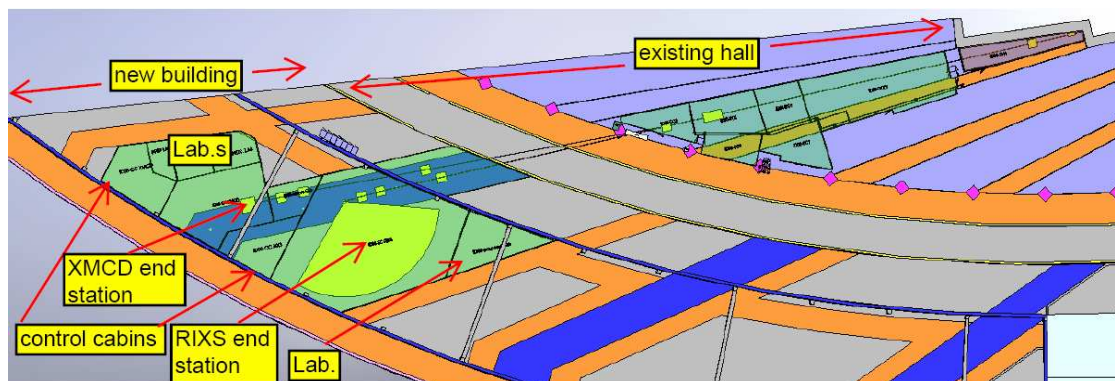
A preliminary design has been produced for the brainstorming with the help of R. Reininger (SAS, LLC) that meets the requirements. A schematic is shown below:



The beamline concept for the RIXS part is based on a variable line spaced grating monochromator for very high resolving power providing $\sim 1 \times 10^{11}$ photons/sec at a resolving power of 5×10^4 with a beam size of $40 \times 3.5 \mu\text{m}^2$ FWHM (h x v). For the fast scanning dichroism branch a constant line grating has been studied with a spot size at the sample down to $70 \times 10 \mu\text{m}^2$ FWHM (h x v) and $\sim 2 \times 10^{12}$ photons/sec at a resolving power of $\sim 5 \times 10^3$ over the entire beamline energy range.

Following the brainstorming the design has been slightly modified to take into account changes to the building and a consequently longer beamline. A double mirror is also envisaged instead of a single one at the start of the beamline for heat load (as pointed out in the original design) and layout reasons. The distances above refer to the new layout. In addition, the recommendation of the brainstorming committee that the beamline should be split before the monochromator and not after as in the first design has been taken into account in producing the budget but the current layout uses the SAS design. The design parameters for the RIXS spectrometer are provided by the Milano group (G. Ghiringhelli/L. Braicovich) based on the existing spectrometer on ID08 and the one they have recently designed for the Swiss Light Source. Space is made for a 10 m scattering arm which can be rotated to change the momentum transfer. Alternatively, a series of spectrometers working in parallel could be used for the same purpose. The spectrometer is based on a variable line density grating and a two dimensional CCD detector (Ghiringhelli et al, 2006). In addition, the possibility of allowing polarisation analysis of the outgoing X-rays should be considered and would greatly enhance the possibilities of the instrument.

The layout of the optics and experimental areas are shown in the figure below with control and support facilities also indicated. This plan was used to provide realistic costs for the infrastructure.



As recommended by the brainstorming committee space is left after the high field magnet end station for user or other beamline end-stations. In addition, any future high DC field magnet would be located outside the building indicated in the drawing and the existing design would allow the beamline to be extended in the future to take advantage of such a development.

End-stations:

Sophisticated end-stations are envisaged to take advantage of the small beams and the space for sample environment that the upgrade extension building provides. For dichroism experiments a new high field magnet (~7 T) with low sample temperatures, possibly vectorial fields and the appropriate UHV sample preparation facilities. It will take advantage of the micron size beams and also allow additional experimental facilities like possibly lasers, pulsed laser deposition for in-situ preparation etc. For the RIXS experiments low sample temperatures and also incorporating high magnetic fields will be very important.

Technical Challenges:

The requirements for very high energy resolution and high flux are very demanding both for the beamline and the resonant inelastic X-ray scattering spectrometer. The recommendation to leave the option open for future detector improvements that might give even higher energy resolution for RIXS also means that the beamline design has to have the potential for higher resolution than considered in the first studies. It is envisaged that, in the spirit of the 15 year old collaboration with the Milano group in this field, that the RIXS spectrometer would be designed in collaboration with this group.

The 10 m rotating scattering arm will represent a significant engineering challenge to obtain the stability, reproducibility and ease of movement of the spectrometer. A viable alternative would be to mount several spectrometers working in parallel: N instruments at fixed angle looking at the same sample would increase the detection efficiency by N and would require a much simpler mechanics to support each instrument. Already two spectrometers (at 90° and 130°) could be an interesting option, to be possibly upgraded at a later time. This needs to be studied to fit within the present budget.

Specific issues are: high quality optics (slope errors as low as 0.1 microrad rms) and efficient cooling of the optics.

For the dichroism measurements the new high field (7 to 9 T) magnet with potentially a vectorial field capability will be a big challenge, as will fast energy scanning and variable spot sizes.

The high field magnet (5 to 8 T) for RIXS experiments will need to allow a large opening angle in the horizontal scattering plane.

Stability in energy and position will need to be carefully considered in the full technical design with particular attention to vibrational problems and thermal stability.

For the RIXS experiments the development in the future of larger CCD detectors or alternative technology will potentially improve the efficiency and ultimate energy resolution that can be achieved.

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