ESRF UPGRADE PROGRAMME

PHASE II (2015-2019)

WHITE PAPER

EXECUTIVE SUMMARY

The science drivers of modern synchrotron science, and therefore of the ESRF Upgrade Programme (UP), revolve around the availability and exploitation of intense X-ray beam providing spatial resolution at the *nano*-scale. This adds a new dimension in the study of innovative materials and new drugs, which need to be understood at the atomic level, and with spatial resolutions in three dimensions extending from the single atom to a few million atoms.

The ESRF UP addresses a new generation of beamlines and studies the optimisation of the X-ray source to produce intense, reliable and stable X-ray *nano*-beams. This programme must be compatible with limits imposed by instrumentation aspects and operation costs and builds upon the existing infrastructure and previous investments in order to minimize construction costs.

The ESRF UP Phase I (2009-2015) has paved the way to the technical realisation of a new generation of beamlines and, with the present paper, to a proposal for a major upgrade of the ESRF storage ring. The new 7-Bend Achromat lattice presented here will allow the ESRF storage ring to operate with a decrease in horizontal emittance by a factor of about 30 and a consequent increase in brilliance and coherence of the photon beam. The increase will be substantially higher than 30 at X-ray energies larger than 50 keV. The new ring will be operated in top-up mode.

The ESRF UP Phase II (2015-2019) outlined in the present White Paper, if confirmed by the Technical Design Report (TDR) to be carried out in the 2013-2014 period and if funded by the ESRF Members, envisages the start of user operation at the end of 2019.

The ESRF UP Phase II (2015-2019) overall budget envelope is in the range of 150 M€. It includes three principal projects:

- The construction and commissioning of the new lattice.
- The construction of four new state-of-the-art beamlines fully exploiting the brilliance and coherence of the new X-ray source.
- An aggressive instrumentation development programme aiming to integrate the technologies required to fully exploit the beamline portfolio in terms of sample positioning and environment, *nano*-focussing, detectors and data retrieval, storage and analysis.

The overall implementation of ESRF UP Phase II (2015-2019) will take place in parallel with normal operation until mid-2018. A long shutdown of about one year will follow to allow the dismantling of the 32 arcs of the existing storage ring, the mounting of the pre-assembled new lattice, and the commissioning of the upgraded ring which is planned to start in early 2019. Users are expected to be back at the ESRF in late 2019.

The ESRF Council has taken note of the White Paper on Phase II of the ESRF Upgrade Programme and endorsed the Management's proposal to start the technical design study, including the reviewing phase of the science case. The White Paper will also be rapidly published on the ESRF Web site and will serve as a basis to develop the scientific case, in collaboration with the ESRF's user community, notably during the forthcoming Users' Meeting on 4-6 February 2013.

TABLE OF CONTENTS

EXECUTIVE SUMMARY 1
1 FOREWORD 3
2 SCIENTIFIC DRIVERS AND REQUIRED ENHANCED X-RAY CAPABILITIES 5
3 ACCELERATOR AND SOURCE UPGRADE 6
  3.1 PROJECT FRAMEWORK AND BASIC CONSTRAINTS 6
  3.2 CONCEPTUAL DESIGN 7
  3.3 PHOTON SOURCE PROPERTIES 9
    3.3.1 Brilliance and coherence 9
    3.3.2 Photons at beamlines 11
    3.3.3 Heat load 12
  3.4 ENERGY EFFICIENT SOURCE 13
4 BEAMLINES 14
5 ENABLING TECHNOLOGY 17
  5.1 TECHNOLOGY DEVELOPMENTS FOR THE ACCELERATOR AND SOURCE 17
    5.1.1 Magnet system 17
    5.1.2 Vacuum system 18
    5.1.3 Radiofrequency system 19
    5.1.4 Diagnostics and instrumentation 19
    5.1.5 Injector upgrade 20
  5.2 TECHNOLOGY DEVELOPMENT FOR THE BEAMLINES 20
    5.2.1 X-ray Optics 20
    5.2.2 Mechanical Engineering 21
    5.2.3 Detectors 21
    5.2.4 Beamline control and data analysis 22
6 ROAD MAP FOR ESRF UPGRADE PHASE II 23
  6.1 TIME SCALE 23
  6.2 FINANCIAL AND HUMAN RESOURCE EVALUATION 24
7 ACKNOWLEDGMENT 24

1 FOREWORD

The ESRF is presently midway through the Upgrade Programme (UP) Phase I (2009-2015).

The present White Paper outlines the main features of the ESRF UP Phase II. It builds on the Science Drivers of the ESRF Upgrade Programme established in 2007 with the publication of the Purple Book and supported by the Council in its Bad Zurzach Resolution of June 2008.

The ESRF UP aims to enable scientists using the ESRF to access a new generation of beamlines providing routine production of intense X-ray *nano*-beams for the analytical study of mesoscopic structures with *nano*-meter spatial resolution. These studies are not attainable by optical microscopy and require unique combinations of real space imaging end microscopy X-ray techniques with established X-ray diffraction, scattering and spectroscopy methods.

The UP Phase I paves the way to this new generation of *nano*-beam X-ray beamlines and substantially improves the reliability, stability and brilliance of the synchrotron source and of the X-ray instruments. The routine availability of this new generation of beamlines will provide unprecedented X-ray imaging capabilities with spatial resolutions in the *nano*-meter regime and time resolution down to the *nano*-second and with major impact in many areas of fundamental and applied science in condensed matter, materials and life sciences research.

The second big challenge of the ESRF UP Phase I is the development of the founding principles for the ESRF UP Phase II, the most important of which being the quest for an upgrade of the source to serve best the science case of the new beamlines.

The present paper is the outcome of preliminary studies and preparatory work on a new generation of storage ring based X-ray sources, whose main characteristic is a substantial increase of the brilliance and coherent fraction of the source as compared to today's X-ray beams: this objective should be reached without compromising the stability and reliability of the ESRF, and without increasing the total radiated power and thus operation, instrumentation development and electricity costs. The driving concept for this "ultimate" machine is to endeavour to reduce substantially the emittance of the stored electron beam, targeting emittance levels capable of providing a fully diffraction-limited X-ray source. Such a limit has been routinely accomplished at the ESRF for the first time in the vertical plane, and has been available to users for one year. The real challenge, however, is to also implement drastic reductions in the horizontal plane, and to make horizontal and vertical emittances comparable. This would correspond to a decrease in horizontal emittance of the order of 500, and a corresponding brilliance increase of the order of 200 compared to existing machines.

Development in accelerator technologies during the last twenty years has lead to many important results featuring new magnet design, innovative vacuum technology, and revolutionizing beam monitoring and orbit feedback systems. These new capabilities and technologies, which were not available or where at their infancy at the time in which the present ESRF storage ring was conceived, provide today a solid basis for the realization of a considerably more advanced storage ring design.

The present paper, based on studies carried out at the ESRF and elsewhere for the realisation of such an “ultimate” storage ring as a new “green field” facility, dwells upon the possible identification of new storage ring lattice design solutions that can be adapted to the existing ESRF storage ring tunnel and which can make efficient use of the existing infrastructure: the same injector system upgraded in the UP Phase I, the same insertion device beamlines, the same bending magnet beamlines, etc... These studies have been very successful and the outcome is indeed a new lattice design, the realisation of which requires the substitution of the 32 arcs of the existing storage ring with 32 new arcs of identical length. The new magnetic lattice reduces the present horizontal emittance of 4nm by a factor of 30 to ~130 pm, whilst preserving the injection system and the 32 straight sections of the existing ring. The consequent increase in brilliance and coherence of the X-ray beam is also a factor of 30. This new source compares very well to an ultimate storage ring design, which would require a further reduction by a factor of fifteen in horizontal emittance to provide an additional factor of five increase in brilliance and coherence. This solution is extremely attractive as it will benefit from the existing infrastructure, thus reducing its implementation costs by at least a factor of ten, and an implementation time by at least a factor of three, when compared to the construction of a completely new facility.

The implementation of the ESRF storage ring upgrade proposed in the present White Paper will maintain Europe’s leadership in synchrotron research by enabling new science and the development of new technologies to the benefit of our society. In particular, the science case supporting the ESRF storage ring upgrade represents a major step forward in synchrotron research, which complements and integrates the new possibilities offered by X-ray Free Electron Lasers (XFELs) and encompasses existing storage ring based synchrotron sources.

Francesco Sette, Director General

2 SCIENTIFIC DRIVERS AND REQUIRED ENHANCED X-RAY CAPABILITIES

The main limitations of X-ray-based experiments at today's synchrotron radiation sources are the poor (transverse) coherence and the limited efficiency of the X-ray optics delivering the X-ray beam to the sample. The latter is directly related to the large horizontal emittance (large horizontal beam size and/or large horizontal opening cone). Whereas synchrotron radiation sources have been optimized rapidly with respect to most of the other fundamental parameters, progress on improvements of these two parameters, horizontal emittance and coherence, has been slow and severely limits the scientific exploitation of synchrotron X-ray beams. Today, particularly in the hard X-ray range, we are still far from the diffraction limit in the horizontal plane.

The aforementioned limitations, resulting in an inefficient use of the photons emitted by the source, affect many scientific applications of synchrotron X-ray beams, employing for e.g. high flux *nano*-meter-sized beams for applications requiring space and time resolution in diffraction, spectroscopy, and imaging. Another direct consequence of the limited source performance is the slow progress in the development of (diffraction) microscopy as compared to the level reached in (transmission) electron microscopy. The coupling of real space X-ray imaging with diffraction microscopy on an atomic length scale is certainly a dream which could become reality, but only at a diffraction-limited light source.

The increased degree of coherence in the X-ray beam from a diffraction-limited source will ultimately allow us to drive the resolution of X-ray based diffraction experiments beyond the limits of the achievable minimum beam size. Coherent diffraction signals encode the intrinsic structure of the probed volume beyond the information on the average structure traditionally retrieved with largely incoherent X-ray beams. An enormous benefit for the more standard applications of synchrotron X-ray beams is the symmetry of the probing X-ray beam delivered by a storage ring based X-ray sources with diffraction-limited performance in both the horizontal and the vertical plane. Today's synchrotron X-ray beams are extremely asymmetric in the horizontal and vertical, resulting in severe limitations in the design of experiments and the achievable resolution in the analysis of materials properties.

Phase II of the UP caters for a similar performance increase of the X-ray source as will be achieved in Phase I with the upgrade of the beamline portfolio. The benefit for the entire scientific community represented at the ESRF will be immediate and will enable experiments on soft and hard condensed matter with unprecedented performance. The full thrust of Phase II of the upgrade will therefore be dedicated to the extensive use of highly brilliant *nano*-beams with the simultaneous application of multiple techniques in order to harvest a maximum amount of information on matter and materials in all relevant time scales. The largely increased level of coherence in the X-ray beam will open a new channel for the determination of micro- and *nano*-structural properties in hard condensed matter as well in biological materials. The application of coherent X-ray beams is today still in its infancy and is driven largely by the new and upcoming X-FEL facilities. The availability of a synchrotron source with a high degree of coherence in its quasi-continuous beams will certainly complement those activities and attract a larger community of users.

The scientific drivers for the UP as defined in the Purple Book remain unchanged with the focus on:

- *Nano*-science & *Nano*-technology
- Science at extreme conditions
- X-ray imaging
- Structural/functional biology and soft matter
- Pump-and-probe experiments and time-resolved science

The proposal for Phase II of the Upgrade in its current form serves all of these areas equally well and will provide European scientists with a unique tool for the exploration of the material world.

3 ACCELERATOR AND SOURCE UPGRADE

Much progress has been made in the framework of UP Phase I in order to increase the brilliance and the reliability of the ESRF X-ray source. However, and as stated in the Purple Book, a recurrent request concerning ESRF beamlines pertains to the reduction of the horizontal emittance. With the strong constraints of reusing the same tunnel and infrastructure, lattice studies carried out at that time did not provide suitable solutions. Today, the situation has drastically changed with all of the efforts that are being made worldwide to develop an Ultimate Storage Ring (USR) design. Present lattice designs and technical developments allow the issue to be re-addressed.

3.1 PROJECT FRAMEWORK AND BASIC CONSTRAINTS

The Accelerator and Source Division is currently studying a new compact lattice based on a 7-Bend Achromat that could replace the existing Double-Bend Achromat.

The ongoing work is performed with the following requirements to:

- Reduce the horizontal equilibrium emittance from 4 nm to about 150 pm
- Maintain the existing ID straight sections in their current state
- Maintain the existing bending magnet beamlines
- Preserve the time structure operation and a multibunch current of 200 mA
- Keep the present injection scheme and injection complex
- Reuse, as much as possible, existing hardware (power supplies, vacuum system, diagnostics, etc…)
- Minimize the energy lost in synchrotron radiation
- Minimize operation costs, in particular the wall-plug power.
- Limit the downtime for installation and commissioning to about one year.

The experience gained during the (accelerator-related) UP Phase I sets a valuable and robust starting point for the complete renewal of the storage ring. The new HOM-damped RF cavities developed at the ESRF will be of capital importance in preventing instabilities induced by the longer longitudinal damping time of the new lattice. The technology of the new RF Solid-State Amplifiers (SSA) installed in the Booster will guarantee the requirements of top-up operation. The conversion of some ID straight sections from 5 to 6 and 7 metres, along with the canting, required the design of new magnets (stronger quadrupoles and permanent-magnet steerers), which paves the way towards the development of the even stronger magnets required for the new lattice. The expertise acquired in state-of-the-art vacuum technology during the last decade (amongst which an in-house NEG coating facility), especially in long straight-section vacuum chambers, represents a solid basis for the design of a new vacuum system in the achromats. The ultra-low vertical emittance (already at diffraction limit) and the orbit stability provided by the new beam positioning hardware and fast orbit feedback are already compatible with the specifications of the new generation of storage rings. Needless to say, comprehensive R&D programmes are necessary for the achievement of all specifications required by the new design.

3.2 CONCEPTUAL DESIGN

The new lattice will fit into the existing facility (in terms of ring circumference, periodicity and beamline positions). It is based on a 7-bend achromat cell displayed in Fig. 1 & 2 and represents a hybrid configuration that takes advantage of the large number of bending magnets (to reduce the horizontal emittance, as implemented in the MAX-IV design) and regions with localized large dispersion (to allow an efficient correction of chromaticity, as in the classical double-bend achromat). In the latest lattice configuration a horizontal emittance of about 160 pm-rad (4 nm-rad today) is obtained thanks to stronger focusing and softer bending magnets (matched to local low values of the dispersion invariant H). The former is obtained by quadrupoles whose gradients have been limited to 100 T/m in order to ensure the feasibility with existing technology. Besides the lower emittance, the net result is an energy loss per turn of about 3 MeV/turn (5 MeV/turn today), which allows a considerable reduction of operation costs due to decreased RF electricity consumption.

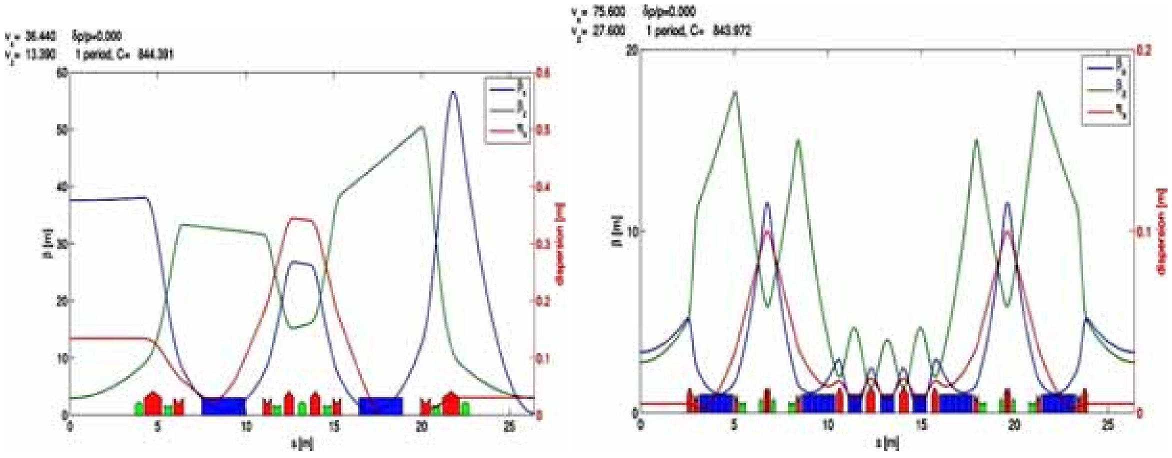


Figure 1: Lattice functions and layout for the existing storage ring (left) and the new design (right).

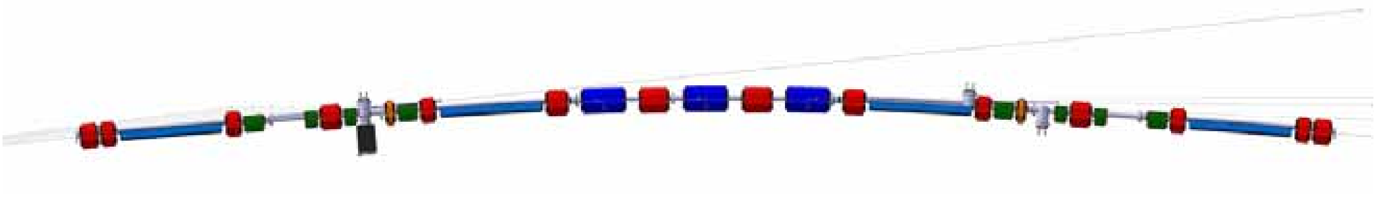


Figure 2: Synoptic of the unit cell (blue: dipole, red : quadrupole, green: sextupole, orange : octupole)

The baseline lattice provides identical optics in all straight sections, with a horizontal β function of 3.4 m, hence removing the alternation of high-β (38 m) and low-β (0.35 m) beamlines. Despite the stronger focusing (both betatron tunes are about twice today's values), chromatic aberrations are comparable to those of the existing machine. Their correction is achieved by two families of sextupoles whose gradients are of about 1.9 kT/m^2, again within reach of existing technology after optimizing the magnet geometry. Geometrical aberrations induced by sextupoles are in turn minimized by a proper choice of their separation and the introduction of octupoles. In order to guarantee sufficient injection efficiency, a dedicated insertion has been conceived to increase the horizontal beta function from 3.4 m to about 12 m or more. The use of independent power supplies for the quadrupoles will guarantee the same level of beta-beating achieved by other existing lower-energy machines, i.e. below 1% peak-to-peak (about 10% today). Preliminary particle tracking studies with 4% beta-beating and about 2% coupling indicate that the nonlinear lattice is close to allowing off-axis injection (Fig.3). The main lattice and beam parameters are listed in Table 1. It is planned to operate the storage ring in constant-emittance mode against variations of the damping induced by Insertion Devices (IDs). These add, on average, about 0.5 MeV of energy loss per turn, with a variation (recorded over one year) of about 0.1 MeV. A dedicated wiggler may be used to stabilize the energy loss per turn and hence the horizontal emittance to 160*(1-0.5/3.0)=133 pm. Even though the design beam current in multibunch mode is set to 200 mA, sub-systems such as RF and vacuum remain tailored to 300 mA.

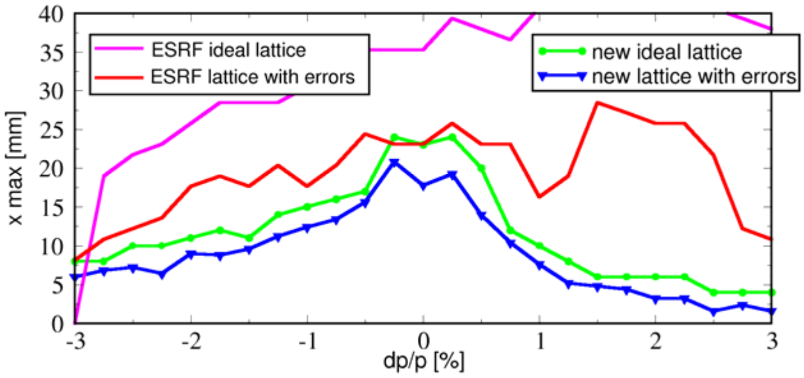


Figure 3: Horizontal dynamic aperture against energy deviation for the ideal lattice (green) and after including errors (blue), (rescaled to equal beta function at injection).

Table 1: Main beam and bare lattice parameters

Parameter	*Existing Lattice*	New Lattice
Energy, E [GeV]	*6.03*	6.03
Circumference, C [m]	*844*	844
Beam current [mA]	*200*	200
Horizontal Emittance [pm ·rad]	*4000*	160
Vertical Emittance [pm ·rad]	*5*	3.2
Bunch length, σ_z [ps]	*13*	11
Energy spread, σ_δ	*$1.06\ 10^{-3}$*	$1.06\ 10^{-3}$
Tune, ν_x, ν_y, ν_s	*36.44 , 13.39, 0.0054*	75.60 , 25.60 , 0.0034
Momentum compaction	*$17.6\ 10^{-5}$*	$8.7\ 10^{-5}$
Damping time, τ_x, τ_y, τ_s [ms]	*7 , 7 , 3.5*	7 , 11 , 7.9
Natural chromaticity, $\xi x0$, $\xi y0$	*-130 , -58*	-97, -79
Energy loss per turn, U0 [MeV]	*4.9*	3.05
RF voltage, V_{RF} [MV]	9	6
RF frequency, f_{RF} [MHz]	*352*	352
Harmonic number	*992*	992
Beta at ID center, βx , βy [m]	*37.6 , 3.0 (high β)* *0.35 , 3.0 (low β)*	3.35 , 2.79
Beam size at ID center, σx , σy [μm]	*413 , 3.9 (high β)* *50 , 3.9 (low β)*	23.5 , 3.7
Beam div. at ID center, $\sigma x'$, $\sigma y'$ [μrad]	*10 , 1.3 (high β)* *107, 1.3 (low β)*	6.9 , 1.3
Beta, beam size and div. at BM	βx= 1,1.6 βy= 42,32 [m] σx =85,113 σy= 13,11 [μm] $\sigma x'$=114,99 $\sigma y'$=0.5,0.4 [μrad]	βx= 0.68 βy= 4.02 [m] σx =13.1 σy= 3.5 [μm] $\sigma x'$=15.4 $\sigma y'$= 0.9 [μrad]

3.3 PHOTON SOURCE PROPERTIES

The large majority of Insertion Devices presently installed are expected to be used in the upgraded accelerator.

3.3.1 BRILLIANCE AND COHERENCE

The improvement in brilliance shall be achieved through a dramatic reduction of the horizontal emittance. Figure 4 compares the brilliance reached with the exiting lattice (plain lines) with that of the new lattice (dashed lines) for different sources.

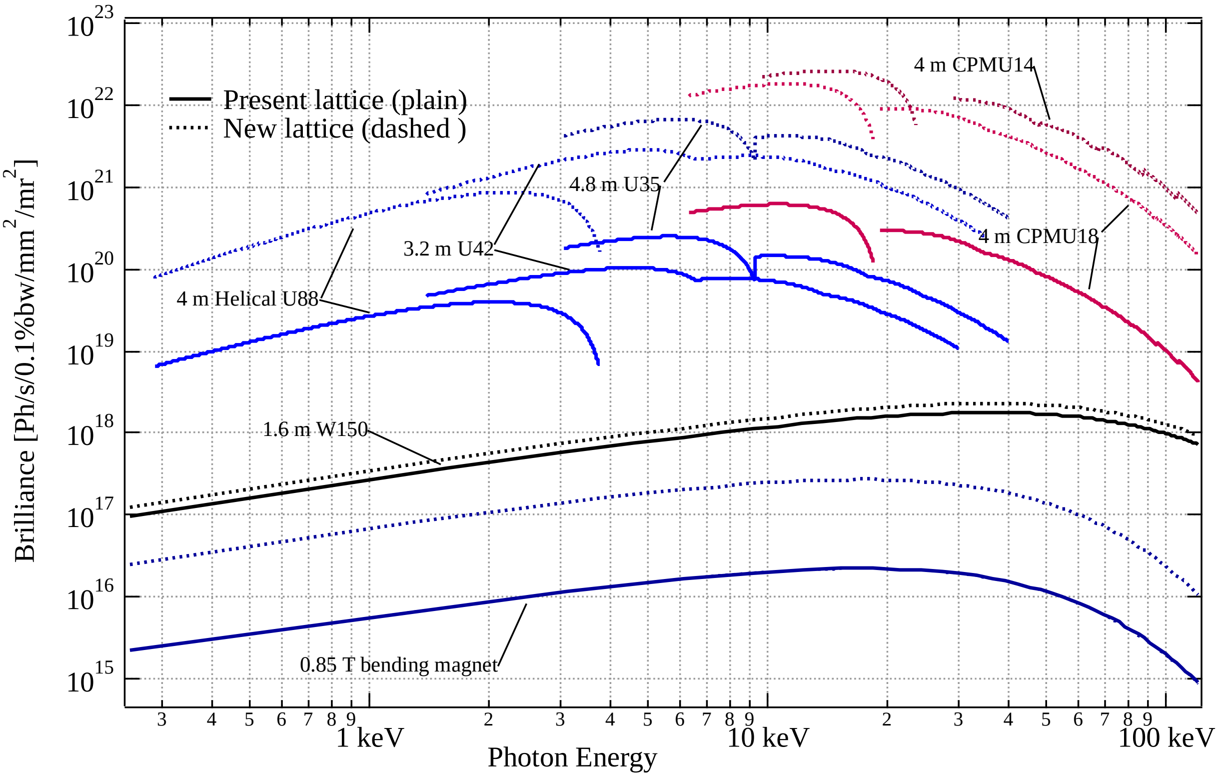


Figure 4: ESRF brilliance for the existing and new lattices

The selected IDs are either presently installed devices or planned devices in the frame of the on-going beamline upgrade. They are separated into different categories: conventional devices, including helical undulators or revolver type undulators operated with a minimum gap of 11 mm (blue), or dedicated devices for high photon energy such as wigglers or the recently developed Cryogenic Permanent Magnet Undulators (CPMUs) with a minimum gap of 5 mm. The technology of CPMUs has now reached a proven mature state. A further improvement of the CPMU technology will be achieved through the use of specific permanent magnet material currently under development in European industry. This will enable the construction of shorter period devices operated at a smaller gap (CPMU14 on figure 4). As far as Bending Magnet (BM) sources are concerned, the exiting 0.85 T dipoles will be replaced by a higher number of dipoles with substantially lower field. In view of restoring a similar spectral range as with present BMs, a local enhancement of the field in the dipoles delivering photons up to 0.85T will be needed. The brilliance of the BM sources is increased significantly as a result of the smaller vertical beta function and horizontal dispersion at the source point achieved with the new lattice. In the wiggler case (W150), the gain is relatively limited because of the depth-of-field effects which dominate the size of the source. For undulator sources, the brilliance is increased by a factor of 16 for photon energy of 1 keV; this factor is more than 26 at photon energies above 10 keV.

The reduction of the horizontal emittance directly improves the transverse coherence with the same gain factor as for brilliance. This can be seen through the coherent fraction defined as:

$fc = \frac{B_n}{B_n^0}$ Where B_n is the brilliance reached on the undulator harmonic, n, with the actual electron beam, and B_n^0 the corresponding ultimate (upper limit) brilliance reached with a filament mono-energetic electron beam. Figure 5 compares the coherent fraction for the present and new lattice as a function of photon energy for different undulators. Note that the electron beam energy spread is taken into account.

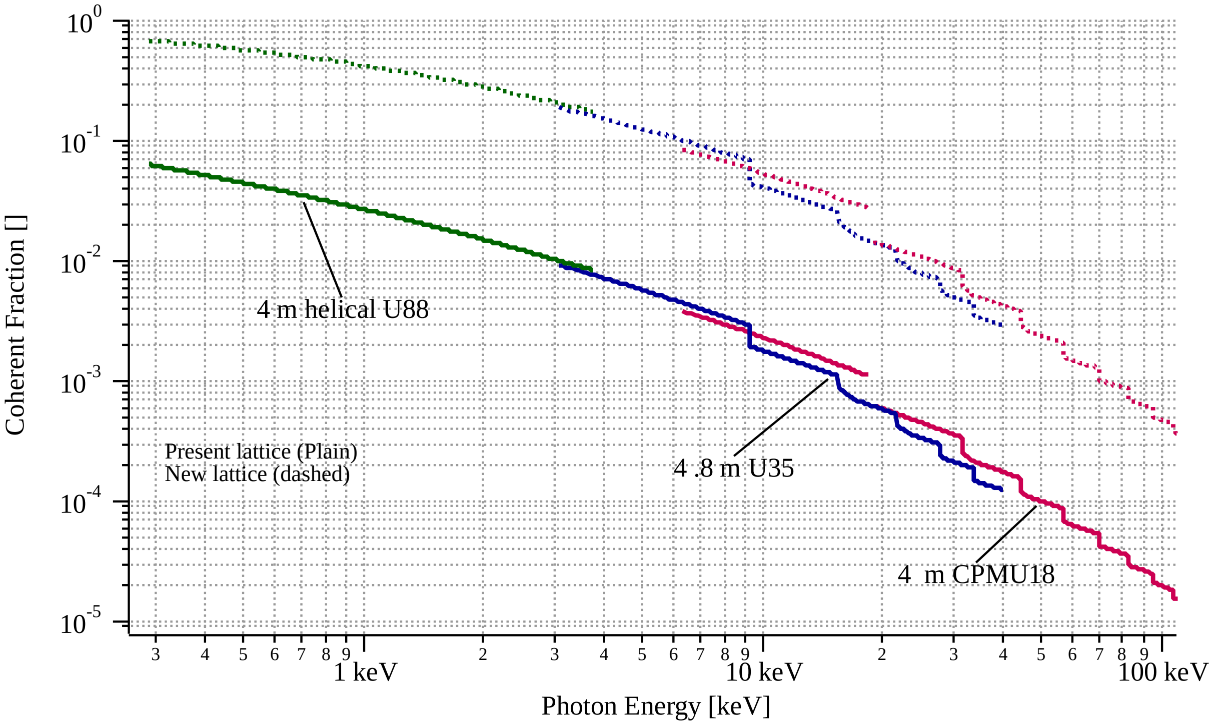


Figure 5: Coherent fraction for the present and new ESRF lattice

3.3.2 PHOTONS AT BEAMLINES

It is useful to look at the on-axis photon flux density (i.e. photon flux per unit surface) collected at the beamline. This is a relevant quantity for beamlines operating with small collecting apertures. Figure 6 shows the increase of photon flux density calculated at 30 m from different sources of the present and new lattice. For bending magnet and wiggler sources, no change in photon flux density is expected.

For beamlines collecting photons over the full central cone of undulator radiation, a relevant quantity is the total flux (i.e. angular spectral flux integrated over all angles). In this case, no change is expected between the two lattices since the total flux is independent of the electron beam emittance and energy. The only difference will be the smaller aperture needed to collect the photons over the central cone with the new lattice. This is barely feasible in the existing low beta undulator sources due to the large aperture needed.

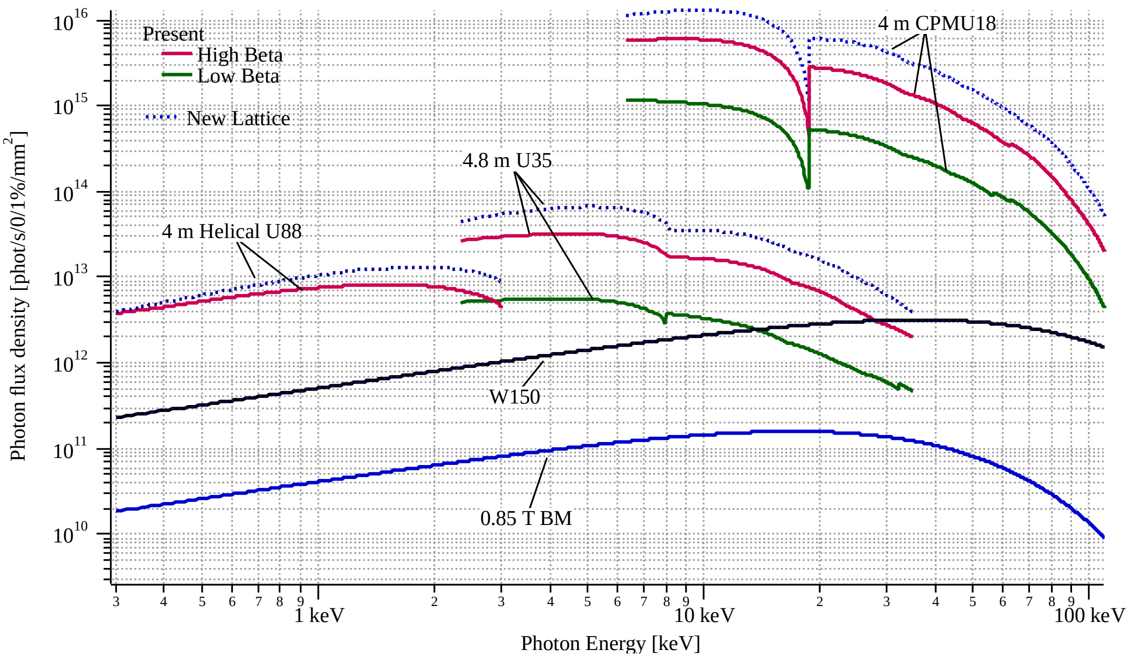


Figure 6: Photon flux density produced at 30 m from different sources for the present and new lattice.

3.3.3 HEAT LOAD

The heat load, and in particular the power density of the white beam, is an important subject for ultra small emittance storage rings. Indeed, for a typical beamline the extracted monochromatic part of the white beam corresponds to a very small fraction of the total incident power which must be eliminated at the first optical components. For an undulator beam, the spatial distribution of the power density is primarily driven by the deflection parameter K of the undulator. For a planar vertical field undulator (the vast majority of undulators), the horizontal angular distribution of the power density has a typical width (rms) of K/γ with γ the relativistic Lorentz factor. In the vertical direction, this width is $1/\gamma$, and as a result the spatial distribution of the power density has a weak dependence upon the horizontal electron beam emittance.

Figure 7 shows the computed power density at 30 m from an undulator with the present (high beta and low beta) and new lattices. The undulator is a 4.8 m long U35 with a K value of 2.3 (gap 11 mm). The new power density is identical to that produced presently with the same undulator in a high beta straight section. In the case of low beta straight sections, the angular divergence of the electron beam (100 μradians) has a visible impact on the horizontal power density but introduces a modest reduction of less than 20 % compared to the high beta case. This may need some more detailed investigation on a case by case basis.

For bending magnet and wiggler sources, there will be no change in heat load between the present lattice and future lattice.

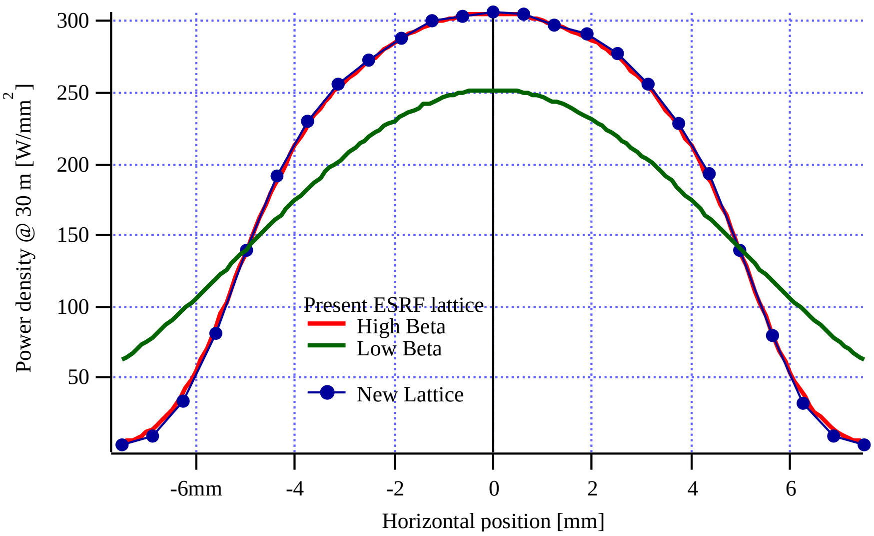


Figure 7: Horizontal distributions of the power density from the white beam generated by a 4.8 m long U35 (K=2.3).

3.4 ENERGY EFFICIENT SOURCE

The new source will be designed with the objective to increase significantly the global energy efficiency in order to reduce electricity consumption. In fact, the cost of electricity currently represents a significant fraction of the ESRF running costs, unlike at the time of the first design (dating back to the end of the 80's). Electricity costs are expected to increase further in the coming decades and consequently improvements in two main domains have been identified:

1) The RF systems will be tailored to the reduced losses per turn, with an expected reduction of about one third with respect to the present RF power consumption.
2) An increase in the efficiency of the production of magnetic fields for the lattice: the main design will be based on conventional electromagnetic magnets, but the possibility of using permanent magnets wherever possible will be investigated.

The overall power consumption of the storage ring, excluding the injector, is expected to be about 60% of the present one. This will counteract the forecasted increase of energy costs over the 10 to 15 years to come. The solutions retained will be based on the global optimisation of capital and recurrent costs over a period of 15 years.

4 BEAMLINES

The first step in the exploitation of the new X-ray source will be the adaptation of the existing beamline portfolio to the performance of the new source. For this purpose an in-depth evaluation of the status of the public beamlines at the end of Phase I of the UP has been performed. The main outcome of this study was that only moderate investments are required in order to benefit fully from the improved X-ray source parameters. These concern mostly the upgrade of mirror systems in the optical train of the beamlines and, in a few cases, the upgrade of the crystal monochromator systems. In the following the main findings of this study are summarized.

Imaging beamlines: The imaging beamlines of the ESRF span many orders of magnitude in energy (from ID21/2keV to ID15A/>200keV) and beam size (from ID16A/10nm to ID17/160mm). Beamlines combining high energy with large beam size will not be affected by the new storage ring (hard X-ray wiggler sources). On the other end of the spectrum are imaging beamlines with very small beams at moderate X-ray energies, such as ID16A, which will benefit from a flux increase up to a factor of 50 at constant beam size with greatly enhanced coherence.

Spectroscopy beamlines: Most spectroscopy beamlines are currently located at high-β straight sections of the storage ring, collecting a large fraction of the useful photons produced by the source on the sample. While in most cases the resolution and the total flux are increasing only moderately, the flux density, i.e. the achievable minimum beam size, will decrease significantly allowing spectroscopic investigations with high spatial resolution as well as with large beams to quantify the average properties of materials.

Diffraction/Scattering beamlines: Most diffraction/scattering beamlines are currently located at low–β sections of the storage ring. Due to the smaller source size at low-β source points, most of the beamlines delivering nanometre-sized beams at the ESRF are located in these sections. In most cases, a large part of the photons produced by the source cannot be collected on the sample owing to the large horizontal divergence, thus rendering *nano*-focusing very inefficient. The new storage ring will not only deliver a total flux increase by more than an order of magnitude, but also enable the focusing of the entire photon beam produced by the undulators into any beam size spanning a range of 5 orders of magnitude, thus increasing the available flux density by up to 3 orders of magnitude and more.

Concepts for four new beamlines will be developed in the coming years with the scientific community. As an example, the case for two new beamlines, a Hard X-ray Microscope (HXM) and a beamline dedicated to Structural Biology, are described.

Samples in hard condensed matter are typically heterogeneous, structurally organized on several length scales and with properties that depend critically on local details. To measure interaction between components, reveal underlying mechanisms, identify critical paths, and optimize process parameters it is essential to visualize the structural evolution directly at the right locations and without sectioning the sample. Uniquely, HXM will provide such data.

The transmission hard X-ray microscope will be a 10-50 keV X-ray equivalent of a TEM. It will enable comprehensive 4D (space- and time-resolved) characterization of the local structure within extended specimens and on the entire scale from 1 mm to, ultimately, 5 nm. A prime application will be 4D mapping of phases, grains, inclusions and stresses as well as individual defects in metals, ceramics, semiconductors and rocks.

The HXM will be based on a new generation of compound refractive lenses. These are specified to provide monochromatic and, potentially, white beam focusing to 10 nm in the 10-50 keV range, and they will serve as a set of objectives, enabling simultaneous full-field microscopy using several different contrast mechanisms. Modalities known from TEM such as diffraction-based dark-field and bright-field imaging will be developed and used to generate 3D maps of crystallography information. Complementary modes will be SAXS imaging, interferometry and section topography. Notably, working distances are long providing ample space for auxiliaries, and the objective in itself acts as a collimator of sorts, vastly reducing the signal overlap between volumes in extended samples.

A guiding principle will be the ability to swap between fast inspection-type mapping on the micron scale over the entire specimen (tomography, 3DXRD) and local studies. Furthermore, for the ultimate spatial resolution, local characterisation based on coherent methods will be explored in order to overcome the resolution limit imposed by the minimally achievable beam size.

The realization of the HXM is critically dependent on the concept of an ultimate 6 GeV storage ring. The 30 times increase in brilliance will enable:

- micron-scale inspection mapping of the entire sample within 10 seconds
- *nano*-focusing to about 10 nm with a superior S/N ratio
- time resolution for 3D local studies in the second to minute range
- the coherent fraction of the beam to be sufficient for 4D studies

In comparison to existing diffraction-based mapping methods (3DXRD, DCT, DAXM), the HXM concept is expected to deliver a spatial resolution that is at least 2 orders of magnitude higher. In-house research performed over the last few years on beamlines ID06 and ID11 in collaboration with several external groups has already demonstrated the feasibility of the HXM concept.

To illustrate the potential impact of the new storage ring on Structural Biology, the likely performance of an improved and extended ID29 is highlighted. ID29 is an ESRF undulator beamline dedicated to the use of anomalous dispersion techniques in macromolecular crystallography with a routinely accessible energy range between 20.0 keV and 6.0 keV (λ = 0.62 Å to 2.07 Å). It is situated on a low-β straight section. Calculations show that implementation of the new storage ring will increase the flux density at the sample by a factor of 25 compared to the current situation. Replacing the mirrors combined with the addition of a new experimental table and a *nano*-diffractometer would improve the functionality of the beamline by an estimated additional factor of 60. Finally, extending the beamline to a length of 100 m could give another factor of 200. In total, combining all possible improvements, the flux density at the sample would be increased by a factor of 300,000, more than 5 orders of magnitude, and that on a fully tuneable, micro focus MAD beamline!

Such an enormous increase in the flux density, combined with a *nano*-sized X-ray beam on the sample position, will allow data collection from the most difficult, very small, weakly diffracting micro-crystals (with an edge-to-edge size of less than 10 μm). However, radiation damage limits the information that can be obtained from such crystals, and therefore will necessitate the use of multiple crystals, similar to what is being explored for XFELs. For the most difficult structural projects the number of samples to be tested may need to be in excess of 1000 to allow collection of a complete diffraction data set. Moreover, the current trend to miniaturize protein crystallization procedures will also result in the increased production of micro-crystals, and thus increase the demand for multi-crystal data collection. Such complex experiments are much more time-consuming (10-20 hours per project) and their success will be critically dependent on the availability of beam time. The development of methods enabling the detailed planning of multi-crystal experiments and the determination of isomorphous subsets from large numbers of samples are already underway.

The quantum leap in performance as calculated for an extended ID29 will change Structural Biology completely. Crystal lifetimes will be of order of milliseconds, and one can expect to collect very few diffraction images per sample. Screening and data collection will be merged and, with such short life times, there will be very limited benefit from cryo-cooling the samples. Some experience with high-throughput, room-temperature sample handling has already been gathered by the initial experiments at the XFELs, offering the possibility for the ESRF to develop sample injection systems closely linked to those being used at the XFELS (e.g. the acoustic droplet ejection method).

It must be mentioned here that the full potential of the new X-ray source can only be exploited with a new generation of instrumentation for sample handling (positioning, throughput, sophisticated in-situ sample environments) and data taking (detectors, fast online data analysis) that is not available today.

5 ENABLING TECHNOLOGY

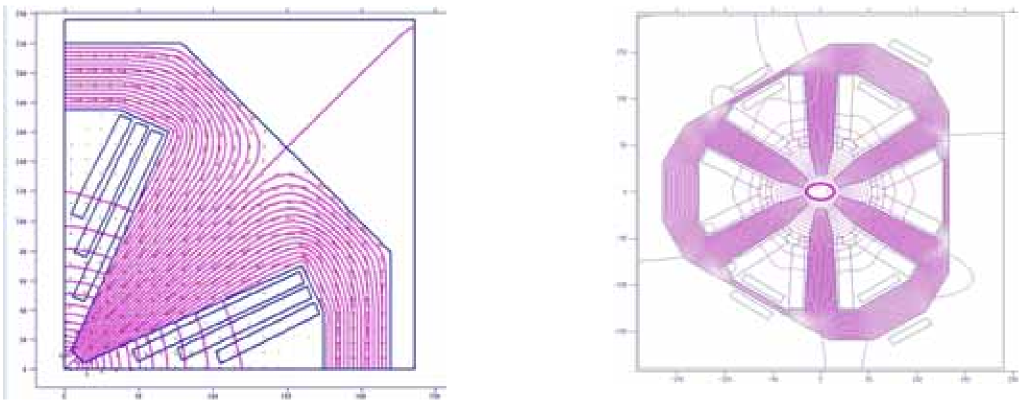
Phase 2 of the ESRF upgrade will generate a large amount of technological developments for both the accelerator & source and the beamlines. The resulting transfer of technology will be beneficial to industry and other synchrotron facilities.

5.1 TECHNOLOGY DEVELOPMENTS FOR THE ACCELERATOR AND SOURCE

5.1.1 MAGNET SYSTEM

The new lattice is composed of 31 magnets per cell, about twice as much as in the present machine. Very high gradient quadrupoles (100T/m) and sextupoles (1.9 kT/m^2) are required, which lead to reduce the magnet bores. Smaller magnetic field volumes represent the first element towards the reduction of both cost and power required. A second aspect shall be an optimized design of electromagnetic magnets to improve their efficiency in the conversion of wall-plug power into magnetic field. To this end, the possibility of combining warm iron-dominated electromagnets with blocks of permanent magnets providing the bulk of the required field is under evaluation. Field quality will certainly be an issue and prototypes will be necessary to validate several concepts under study.

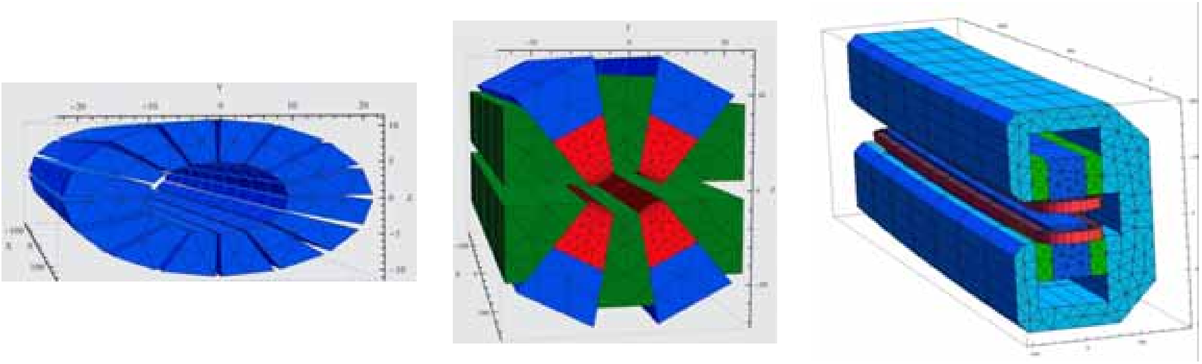
The four long dipole magnets require a longitudinal field gradient. The three short dipoles comprise strong transverse gradients: they are horizontally offset quadrupoles open externally for the extraction of the X-ray beam along vacuum antechambers. High-gradient quadrupoles are extrapolated from the design of the 7 m straight section magnets by reducing the bore radius from 33 mm to 13 mm (Fig 8.a). A redesign of the magnetic poles at the saturation limit of high power grade iron available on the market is needed. The shape of the yoke shall cope with the extraction of the X-ray beam. A special three-fold symmetric design for the (otherwise six-fold symmetric) sextupoles is necessary to extract the X-ray beam (Fig 8.b). The thin return yoke enables flexible correction functions as in today's sextupoles.



(a) (b)

Figure 8: Electro magnets: quadrupoles (a) and sextupoles

High performance permanent magnet (PM) design for dipoles and multipoles will commence in parallel with the design of conventional electromagnets (Fig. 9). Using PMs may lead to better performance, more compact design and significant energy savings. PMs are good candidates for small aperture multipole magnets. The key points of such designs are the minimization of the quantity of magnetic material, the development of a tuning system and the possibility to “shim” the magnetic field. PM dipoles will be equipped with a small-range coil-based tuning system. Fixed-field PM steerers have been successfully installed this year in the storage ring. The magnetic performances of higher-order PM multipoles are very attractive. The dimensions of sextupole magnets would be dramatically reduced by using a hybrid PM-coil design.



(a) (b) (c)

Figure 9: Permanent magnets: modified Halbach quadrupole (a), hybrid quadrupole (b), hybrid dipole (c).

For the dipoles, a hybrid configuration using permanent magnets, high power grade iron, copper coils, and mechanical adjustment also looks promising. This type of solution enables correction due to the thermal behavior of the magnets as well as lattice trimming in all the cells. It is envisaged to start PM design and prototyping in 2013.

5.1.2 VACUUM SYSTEM

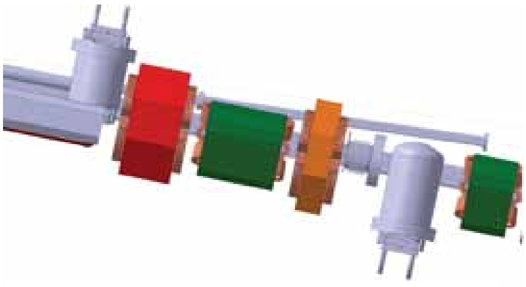


Figure 10: Vacuum chambers outline with front end

The vacuum system will be dominated by chambers with low vacuum conductance due to the space constraints dictated by the magnets. The main chambers will be made from extruded aluminum profiles; where necessary a passage to stainless steel will be assured by explosion bonded interface pieces. More complex chambers requiring the connection of vacuum pumps, gauges and residual gas analyzers will be made of stainless steel. Vacuum pumping will be provided by non-evaporable getter (NEG) coating all along the electron beam path. Non-getterable gases will be pumped by sputtering ion pumps, an integrated solution for the lumped pumps combining a small sputtering ion pump and a NEG cartridge are under study. The radiation of the dipole magnets will be preferably collected by lumped absorbers; as the power generated by a single dipole magnet is lower than as for the actual machine, these absorbers will be a downscale of two prototypes already in place on the present storage ring. A solution combining the lumped vacuum pump and absorber on one flange is being investigated. The antechamber design of the principal vacuum chambers assures that the photon beam goes to the beamline; the antechamber provides additional surface to be covered with NEG in order to have more distributed pumping speed. This design requires a large connection flange for the vacuum chamber, which may allow the re-use of the existing gate valves which would have to be modified. The vacuum instrumentation layout will be oriented on the present one with four total pressure gauges and one residual gas analyzer gauge per unit cell and two total pressure gauges and one RGA per insertion device sector.

5.1.3 RADIOFREQUENCY SYSTEM

Figure 11: HOM damped cavity

The low fields in the bending magnets result in a reduction of the synchrotron radiation loss from 5.4 to about 3.5 MeV/turn, including ID radiation. The longitudinal damping time increases from 3.5 to 7.9 ms. The momentum compaction factor is divided by two. As a result, the new machine will only need between 5 and 6 MV of RF voltage instead of presently 9 MV to guarantee an RF energy acceptance between 3 % and 4 %, and the beam power at the nominal current of 200 mA will drop from 1100 kW to 700 kW. The new lattice will be twice as sensitive to longitudinal coupled bunch instabilities. The five-cell cavities will therefore no longer guarantee stable operation at 200 mA. The required stability will be obtained replacing the five-cell cavities with 12 HOM-damped single cell cavities developed in the frame of the UP Phase I (Fig 11). Each one will require about 100 kW of RF power to operate at 200 mA. The existing klystron transmitters and the three Solid State Amplifiers (SSAs) that are being installed in UP Phase I will provide the necessary power. The implementation of a harmonic RF system for bunch length manipulation is envisaged.

5.1.4 DIAGNOSTICS AND INSTRUMENTATION

The number of BPMs needs to be increased from 7 to 12 per cell because of the increased phase advance. The present electronics for data acquisition and processing, newly installed in 2009, will be reused. The additional BPM units will be equipped with a renovated version of these electronics since the existing system will be obsolete at that time. The BPM blocks will be made out of aluminum and positive experience has already been gained at the ESRF with such design for test purposes. The orbit correction and stabilization will rely on the above BPM system and the orbit steerers combined in a feedback system similar to that recently put into full operation. It will provide full damping of both the effect of the gap variations of the insertion devices and any transverse AC (up to 100Hz) motion of the beam position, thereby providing the users with an ultra stable X-ray beam. The emittance measurements will be performed at numerous positions around the ring by using the available bending magnet beamports that are not equipped and used for a beamline. With the well established technique of X-ray pinhole cameras, a total of 15 to 20 devices could be installed, fully contained inside the ring tunnel, while providing the necessary measurement precision in both transverse planes.

5.1.5 INJECTOR UPGRADE

The present ESRF injector will be used to inject in the new storage ring. The upgrade of the injector as part of the UP Phase I will meet the requirements for the new machine, in particular the top-up operation. It is described here for completeness but will not require additional resources from Phase II. Ramped power supplies allowing a 3-4 Hz cycle of the booster magnets will replace the existing 10 Hz resonant one, in order to enhance stability and allow shaping of the accelerating ramp. The RF of the booster has been recently upgraded to solid state amplifiers. The new design will then make possible the implementation of bunch cleaning, with the same quality in the booster, instead of the present technique performed in the storage ring. The orbit stability in the booster will also be enhanced by implementing an orbit correction scheme at high energy and by improving control of the beam trajectory in the transfer line between booster and storage ring. Timing will also be redesigned to allow multiple injection/extraction within one booster cycle. A consolidation programme to guarantee the reliability and redundancy is in progress as well, which will also benefit the new machine.

5.2 TECHNOLOGY DEVELOPMENT FOR THE BEAMLINES

The expected source properties associated with the new science drivers will require not only state-of-the-art instrumentation but also development and implementation of innovative strategies. Phase II will offer a unique context to strengthen developments initiated in Phase I and to address new challenges. Overall, the ESRF intends to undertake an aggressive instrumentation development programme aiming to integrate the best technologies required to fully exploit the ESRF beamline portfolio in terms of sample positioning and sample environment, optics, detectors and data retrieval, storage and analyses.

5.2.1 X-RAY OPTICS

The majority of the undulator beamlines should reap immediate performance benefits from the improved source characteristics. Moreover, the move towards operation in the top-up mode will alleviate drifts of optical systems resulting from variations in the absorbed power of upstream components which can occur during operation in current-decay mode. Nevertheless, in many cases, realizing the full potential of the upgraded source will require the development and implementation of improved quality beamline optics. The preservation of the improved horizontal beam emittance following propagation along the beamline will be particularly challenging.

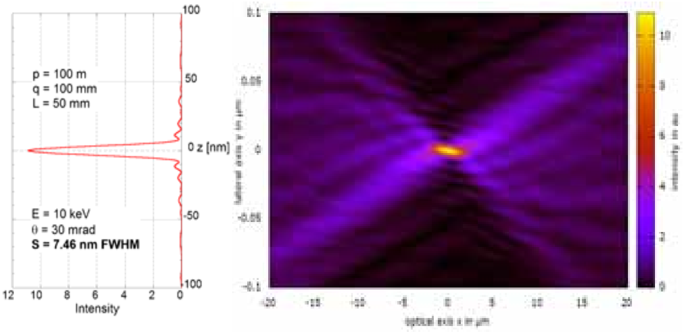


Figure 12: Simulated intensity distribution near the focal spot of a W/B$_4$C multilayer-coated focusing mirror

Reflective, refractive and diffractive optics will continue to be incorporated in the beamline optical designs which will need to be optimized individually according to experimental requirements using advanced design tools (see e.g. Fig.12). There is scope to improve the performance of most classes of X-ray optics and, in the majority of cases, promising pathways to achieving the necessary optical quality have been identified or are already being explored. Meeting the improved specifications will require increased investment in optical modeling, manufacture, testing facilities and integration through in-house and external development programs. For the latter, joint technology developments with industrial suppliers and/or external research groups are envisaged. For applications exploiting the improved transverse beam coherence, clear opportunities for synergetic developments with the new X-ray FEL sources exist.

5.2.2 MECHANICAL ENGINEERING

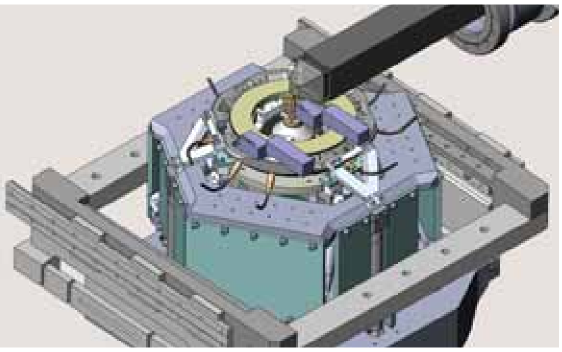


Figure 13: UPBL4 *nano*-imaging end station

The low horizontal emittance of the source and the high degree of coherence of the X-ray beam leads to more stringent requirements upon component stability and positioning and sample environments. The investments made during the Phase 1 (e.g. extension of the capabilities of the precision metrology laboratory, creation of a high precision assembly facility), together with the expertise and experience gained with for example the UPBL4 NI end-station project will serve as a basis for phase 2 beamlines. In order to address the new technical challenges in the field of *nano*-metric precision, the existing group of specialized engineers fully dedicated to high precision projects will be reinforced with a focus on mechatronics, including a new R&D program on real-time correction of positioning errors requiring state-of-the-art *in-situ* metrology associated with advanced control methods. The most challenging instrumentation will rely upon the availability of advanced modeling techniques to address thermal and dynamic stability performance. The current effort in the developments of innovative sample environments will be pursued and reinforced with a particular focus on their integration in the overall design of end-stations.

5.2.3 DETECTORS

The new source properties will translate into new opportunities in terms of both time and spatial resolution. The increased flux will promote the use of higher acquisition-rate detection systems. Exciting scientific opportunities will become possible with the emergence of a new generation of time-resolved detectors combining nanosecond temporal response and 2D ability. New 2D detectors with reduced pixel size and improved radiation hardness will be addressed in the Phase 2 program. As an example, small-pixel hybrid detectors, (5-30 µm pixel size) are very attractive for scattering applications and silicon hybrid pixel detectors in integration mode are considered good candidates for use in the 5-15 keV energy range. Current efforts to improve detector efficiency for hard X-ray detection will be pursued. In particular, in-house developments on thin scintillators and High-Z semiconductors for hybrid pixel counting detectors have been initiated and will be consolidated in Phase 2. CMOS imaging sensors exhibit interesting features for fast imaging cameras which allow ultrafast process to be recorded owing to electronic shutter and fast readout. *CMOS Monolithic Active Pixels Sensors* (MAPS) are particularly interesting candidates to overcome some limitations of CCD cameras, allowing reduced exposure times, larger field of view and higher dynamic range (see fig. 14). Detector developments will require significant long-term investment, over a minimum of five years and, owing to complexity and diverse requirements, favor collaborative efforts with X-FELs and other synchrotron facilities.

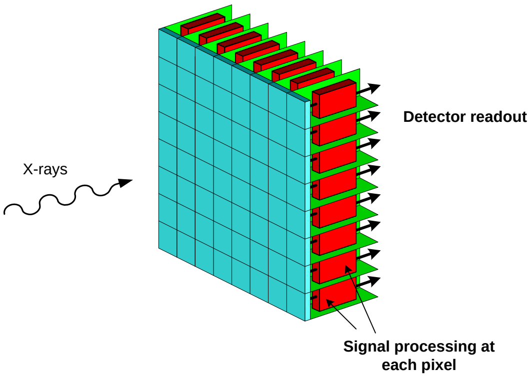


Figure 14: Large format high-dynamic range MAPS sensors.

5.2.4 BEAMLINE CONTROL AND DATA ANALYSIS

The source upgrade will enable more complex experiments with much higher data rates. A major upgrade of the beamline control system software will be necessary to exploit fully the new instrumentation. Initiated in Phase 1, the modernisation effort could be fully deployed during the long shutdown of 1 year offering a unique opportunity during the lifetime of the ESRF for this. On-the-fly scanning and zero-dead-time experiments will be generalised. The LIMA based framework will be extended to support the wide variety of the new 2D detectors which will be installed on beamlines. LIMA will be pushed to higher data rates which will imply new file formats and faster data writing. The writing of metadata will be generalized to all beamlines to enable online data analysis. Today, users often face a data bottleneck i.e. data are produced at a faster rate than users can analyse. This is largely due to a lack of adequate online and offline data analysis software. To cope with this issue, it is intended to boost investments in this field during Phase 2. Online analysis will be addressed first to improve the quality of data taken during experiments. The work started during Phase 1 to store the metadata needed for online analysis in a metadata catalogue will be generalized to all beamlines and will facilitate data management e.g. automatic archiving of raw data. Existing offline scientific software will be improved to boost execution speed and to address new needs. For instance, analysis software will need to cope with the ever increasing number of combined measurements, where cross-correlations hidden in the data coming from individual experimental techniques will have to be unveiled and understood with the help of suitable computational tools.

6 ROAD MAP FOR ESRF UPGRADE PHASE II

6.1 TIME SCALE

Upon the approval of the White Paper, a Technical Design Study (TDS) phase of approximately eighteen months will be launched to prepare a full report. This TDS will be submitted first to the Accelerator Project Advisory Committee (APAC) – to be created by the ESRF Council - for comments, amendments and discussion and then to the ESRF Council for approval by the end of 2014 and for launching the procurement phase in 2015. The time scale of the whole storage ring upgrade project should fit within the Phase II of the UP. The machine will be stopped for approximately one year as from August 2018 (5 months in 2018 and 8 months in 2019), including the two long summer shutdowns. This long shutdown will be used for the dismounting and installation of all equipment in the tunnel (11 months) and for commissioning (2 months). Beam should be back at the end of August 2019 for the restart and commissioning of the beamlines (2 months) and then back to external users by the end of 2019.

26 Nov 2012	White paper presented to Council, start of technical design phase
End 2014	Completion of TDS
Earlier 2015	Engineering design, calls for tender
Earlier 2017	Vercors building completed, assembly and preparation starts
Mid 2018	Begin of shutdown for installation of the new storage ring
Mid 2019	Begin of commissioning phase
End 2019	Start of user mode, 2 new upgrade beamlines in Chartreuse
End 2020	2 new upgrade beamlines in Vercors

Figure 15: Time scale of the ESRF Upgrade Phase 2

A large storage and preparation building is mandatory for the assembly, test and qualification of the 32 arcs. The absence of such premises was a bottleneck for the projects done in the Phase I. The construction of the Vercors building, initially foreseen for Phase I, would be an excellent solution considering that its architectural study is essentially done and that this building could later be used for the construction of new long beamlines as initially planned. This building (4,400 square metres) should be ready at least 1.5 years prior to the start of the one year long shutdown.

The ESRF should be ready to launch the first calls for tender at the beginning of 2015, with manufacturing, construction and test periods from mid-2015 to the beginning of 2018. The Technical Design Study should be ready and endorsed by the APAC by the end of 2014. Prototyping and R&D will start right from the approval of the present White Paper in order to be used for the preparation and validation of the TDS report.

The construction of four new beamlines will be divided in two phases. Two beamlines will be built in the Chartreuse experimental hall during the one-year shutdown, while the other two will be constructed as soon as the new Vercors building is freed of the new storage ring equipments.

6.2 FINANCIAL AND HUMAN RESOURCE EVALUATION

At this stage of the project, only preliminary estimates of cost and manpower can be made. A first evaluation of all the tasks and the associated budget has been performed on the basis of the recent accelerator and beamline projects realized for UP Phase I. Information will be published once the preliminary data has been consolidated.

7 ACKNOWLEDGMENT

The ESRF Management put together the present paper in a very short time since in early spring 2012 the scientists and engineers of the ESRF Accelerator and Source Division indicated new exciting and, at the same time, realistic possibilities for a major storage ring upgrade. This paper has been possible thanks to the commitment, enthusiasm and motivation of many ESRF staff who have worked very hard to provide solid material to substantiate the present proposal for the ESRF UP Phase II. The ESRF Directors fully acknowledge the ESRF staff for their outstanding contributions to the preparation of the present paper.