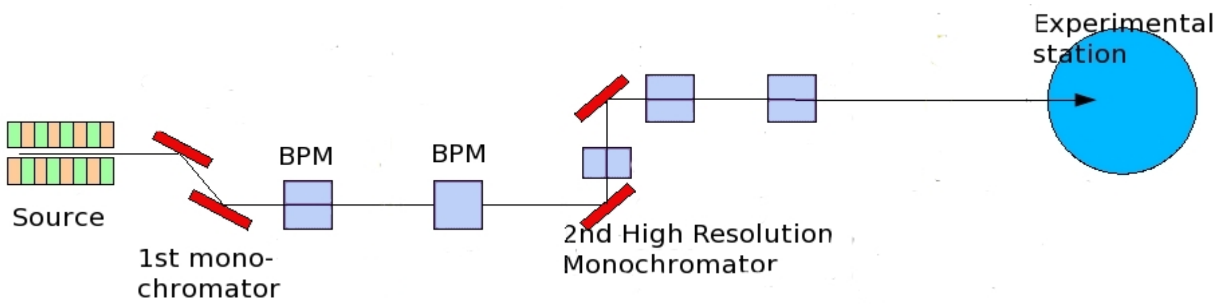
1. ***Proposed Optical Configurations:***

1.1. High-Resolution Raw Configuration:



This configuration is specially adapted for Coherence.

The first optical element of the beamline will be a liquid nitrogen cooled double-crystal silicon monochromator. The monochromator includes two pairs of crystals, with symmetrical (1 1 1) and (2 2 0) reflections. The former pair can be used for preliminary monochromatization in the energy range from 5 to about 25 keV, while the latter one can be best operated in the higher energy range. Two beam position monitors right after the monochromator are used to stabilize the x-ray beam by means of horizontal and vertical position and direction (accuracy better 5μm in position and better 1μrad in direction).

The second monochromator will be a set of interchangeable channel-cut Si crystals with (1 1 1), (1 1 0) and (3 1 1) surface orientations will allow a wide choice of intensive reflections. Depending on the combination of reflections employed, the divergence of the beam can vary between 0.5 μrad to the full 5 μrad coming from the source. Simultaneously, this monochromatization system ensures an energy resolution $\Delta E/E \sim 2\ 10^{-4} - 5\ 10^{-5}$ in the whole energy range. The same double channel-cut monochromator provides a high angular collimation. The secondary monochromator should preferably be placed near to the sample position for small beam cross-sections.

The second monochromator is a large offset monochromator (LoffsMono). It is a specially designed device that:

1) Lifts the beam up by a desired height. This is especially import because for the desired scientific surface purposes it is necessary to have a large diffractometer that could allow to put large sample environments.
2) To increase the resolving power of the x-ray beam. Depending on the combination of reflections employed, the divergence of the beam can vary between 0.5 μrad to the full 5 μrad coming from the source. Simultaneously, this monochromatization system ensures an energy resolution $\Delta E/E \sim 2\ 10^{-4} - 5\ 10^{-5}$ in the whole energy range.

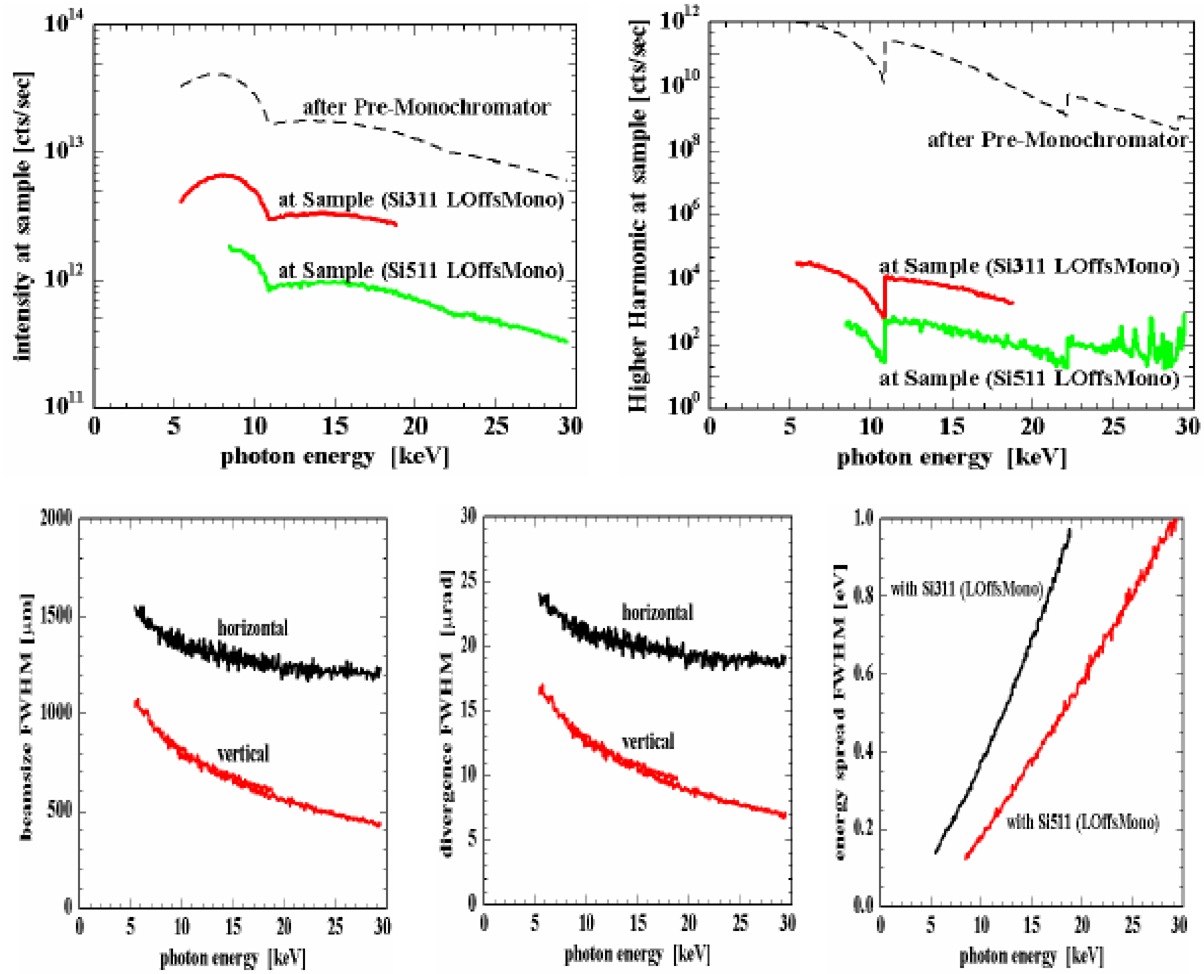
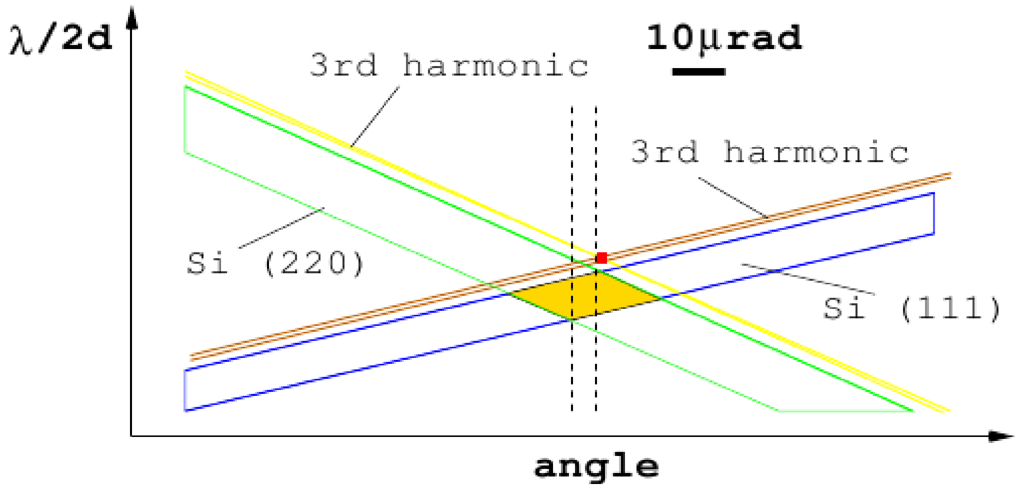


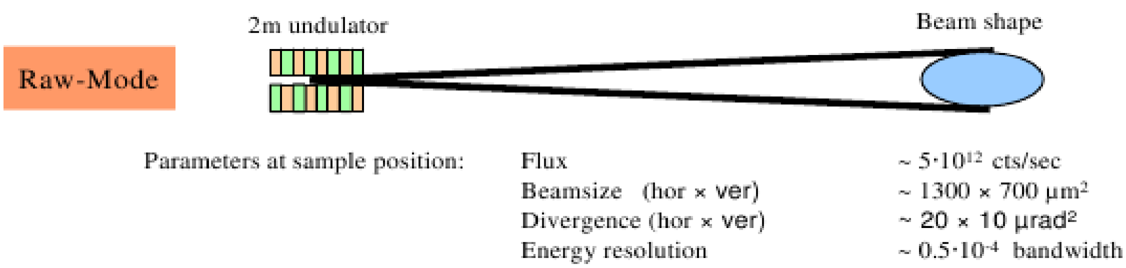
Figure: Parameters of the x-ray beam at the sample position using the raw-mode at HighRes. Top left the intensity in counts per second. Top right the contamination due to higher harmonic photons in counts per seconds. Bottom left the beam sizein µm (FWHM), bottom center the divergence in µrad (FMHW) and bottom right the energy resolution in eV.

3) To remove the higher harmonic contamination of the x-rays. Thus, this crystal arrangement suppress the higher harmonics (next figure). This configuration has the advantage with respect to the most used monochromator + mirror configuration that avoid the use of a perfectly flat (low roughness) mirror surface that in other case could highly reduce the beam coherence. At the cost level it is estimated that both configurations should be almost the same.

Figure: Suppression of higher harmonics by Bartels type monochromator. The du Mond diagram presents, as an example, a case of Si(111)/Si(220) reflection pair at 8 keV, with the third harmonic at 24 keV. The higher harmonics are visible only in a narrow angular interval, marked by the red spot. Already a minor detuning of crystals allows to suppress the harmonics by a factor of 10^{-4} or better. The dashed lines mark the angular interval, where the transmitted beam will pass without a loss of intensity.

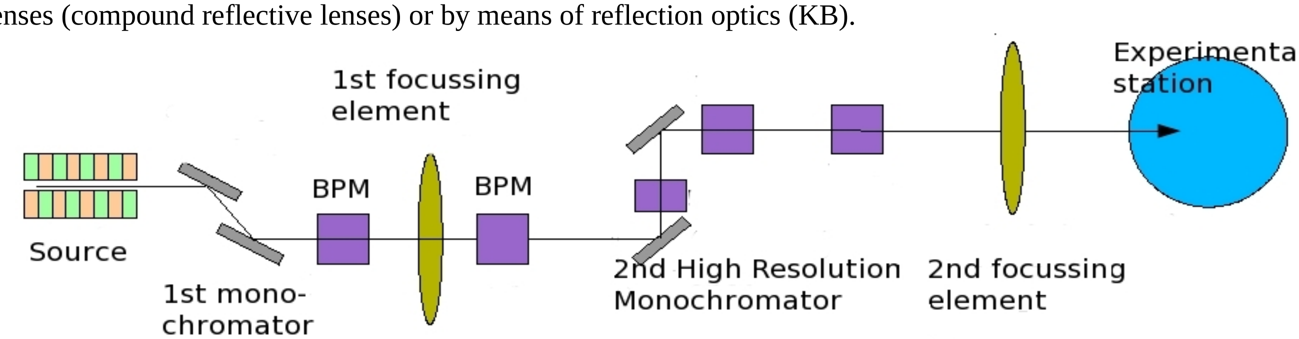


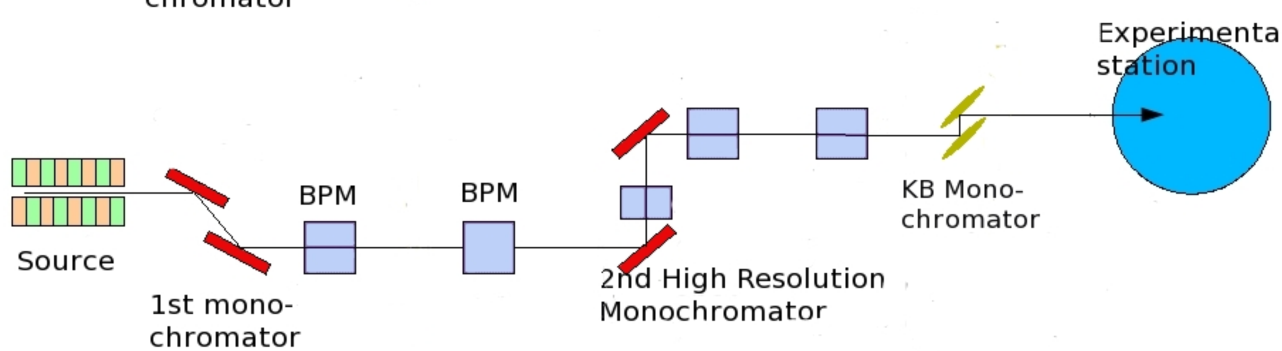
The first estimation of beam parameters are at this operation mode are:



1.2. High-Resolution from collimation to microbeam passing through focusing Configuration:

In other to get a microbeam, necessary for microfocus Surface X-ray diffraction experiments and microcrystals diffraction, two methods are mainly proposed in literature: by means of transmission lenses (compound reflective lenses) or by means of reflection optics (KB).

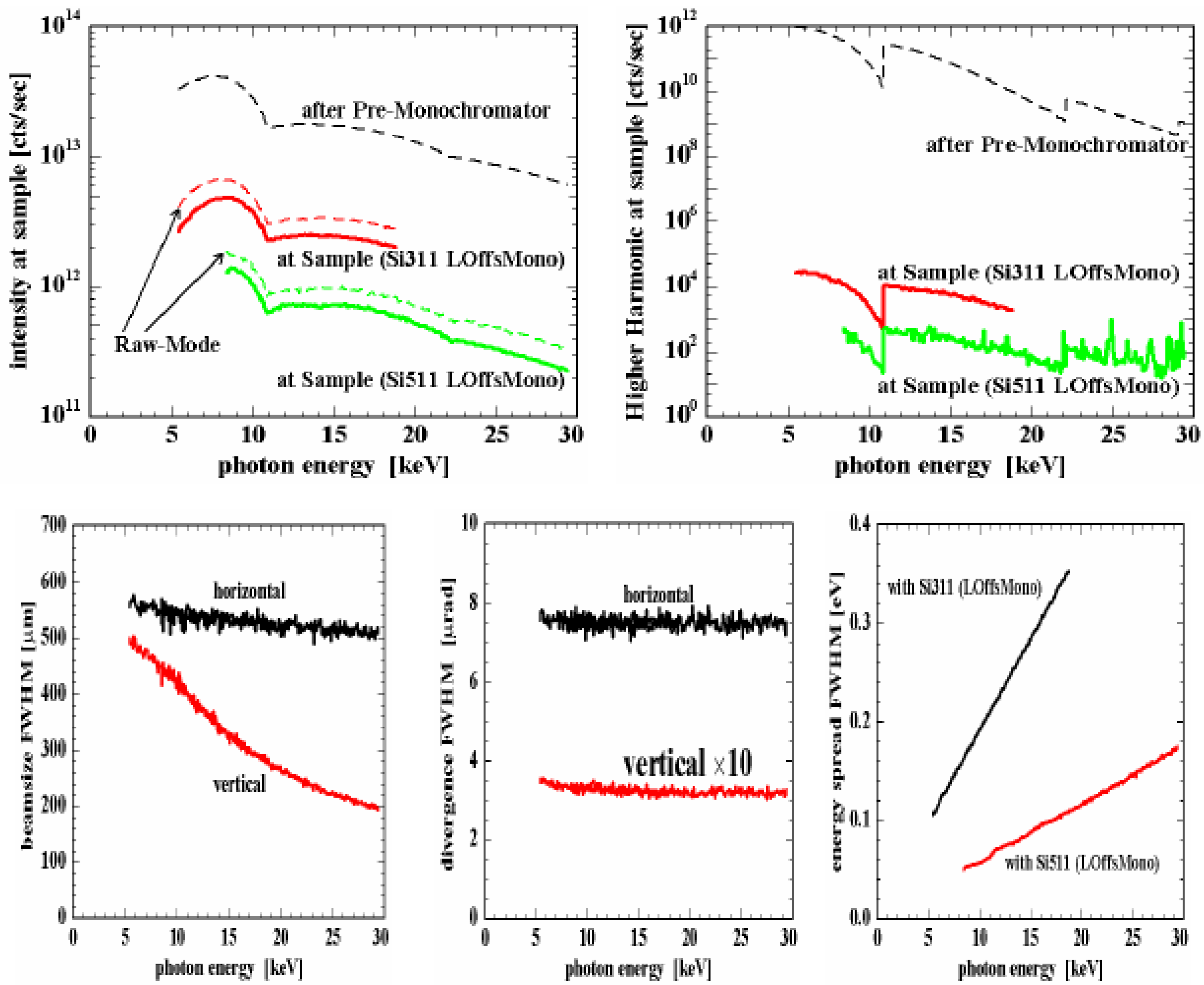




One of the main advantages that gives the transmissions lenses (top figure) is the that not changes the beam position at the experimental hutch that increases the compatibility of the microfocus and the parallel-beam configuration. This is the reason that we propose the use of this optical configuration for the beam-line. Furthermore, optional compound refractive lenses can be used to collimate the x-ray beam (compensation of divergence) or to slightly focus the beam without arriving to the microfocus configuration. Both reasons determine that we prefer the first solution based on compound refractive lenses.

*1.2.1. **The collimation-mode***

In the collimation-mode the CRLs located in the optics hutch are chosen in such way that the beam divergence is minimized. The CRLs close to the sample position are not used. With this configuration the beam is parallel and it is obtained the best resolution in the reciprocal space. This configuration should be the most used for surface x-ray diffraction of low scattering power system.



*1.2.2. **The focusing-mode***

In the focusing-mode the CRLs located in the optics hutch are chosen such way that the beam size at the sample is minimized. The CRLs close to the sample position are not used. In the focusing-mode moderate focusing is realized with still very good resolving power in reciprocal space. This configuration should be used for surface located problems and medium size crystals experiments.

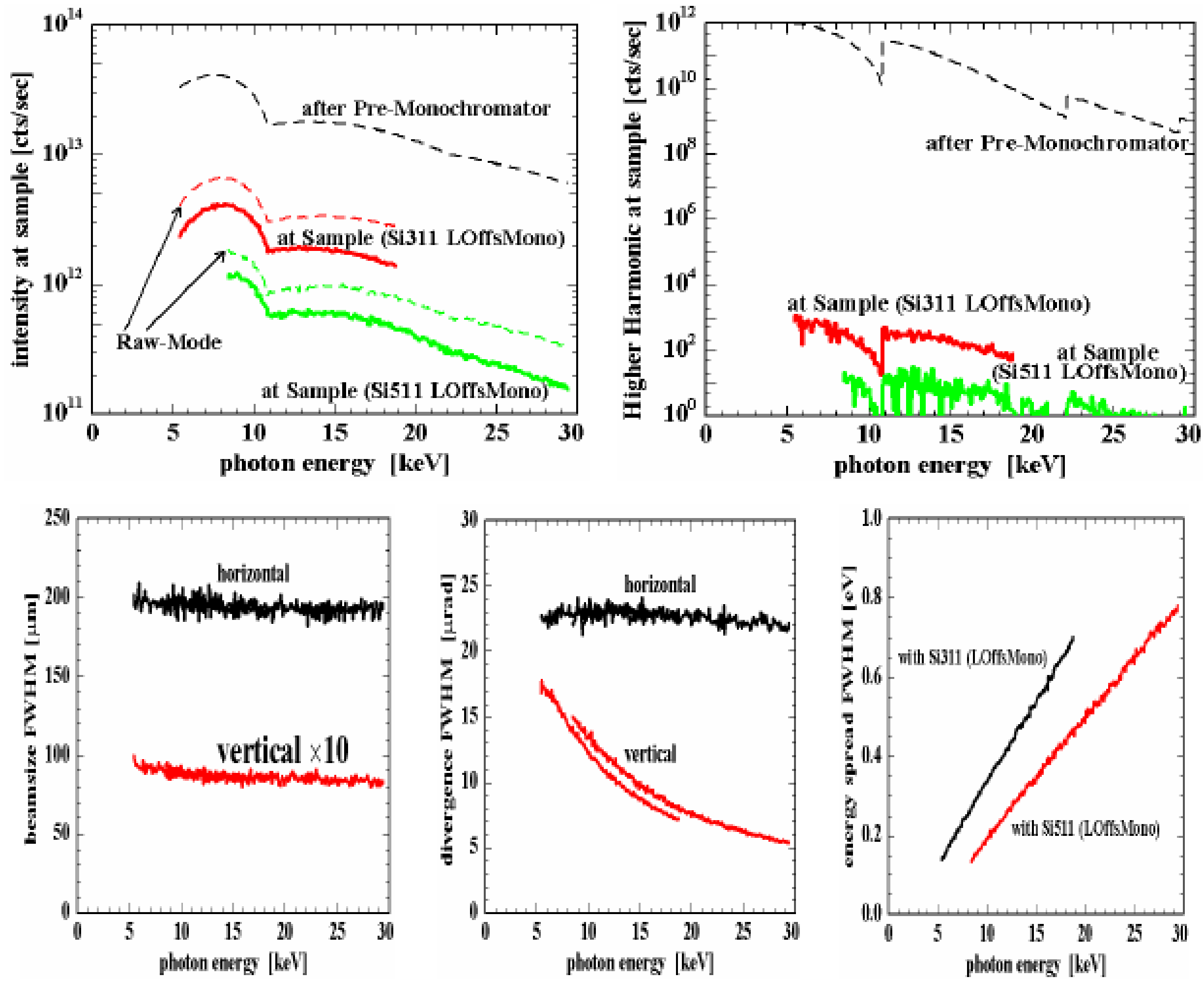


Figure: Parameters of the x-ray beam at the sample position using the focusing-mode at HighRes. Top left the intensity in counts per second. Top right the contamination due to higher harmonic photons in counts per seconds. Bottom left the beam size in µm (FWHM), bottom center the divergence in µrad (FMHW) and bottom right the energy resolution in eV.

*1.2.2. **The microbeam mode***

In the µ-mode the number of CRLs located in the optics hutch are chosen such that the divergence of the beam is minimized (collimation). The CRLs close to the sample are chosen such that the beam size at the sample is minimized. In that case we lose in reciprocal space resolution but the best real space resolution. This is especially adapted for resolving surface micro-structures (i.e. micro-strippes arrays, micro-wires arrays in surfaces, ...) and micro-crystals.

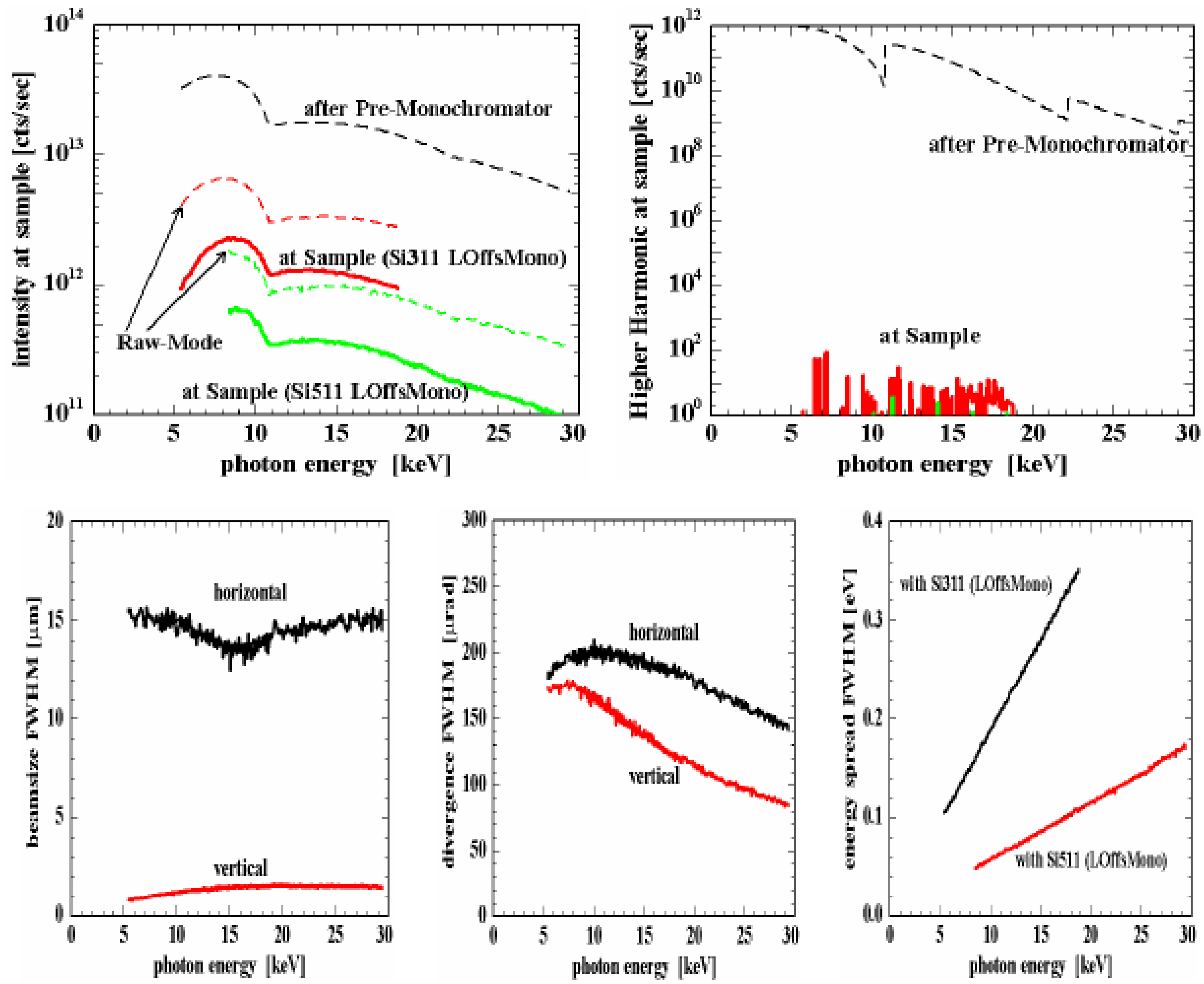
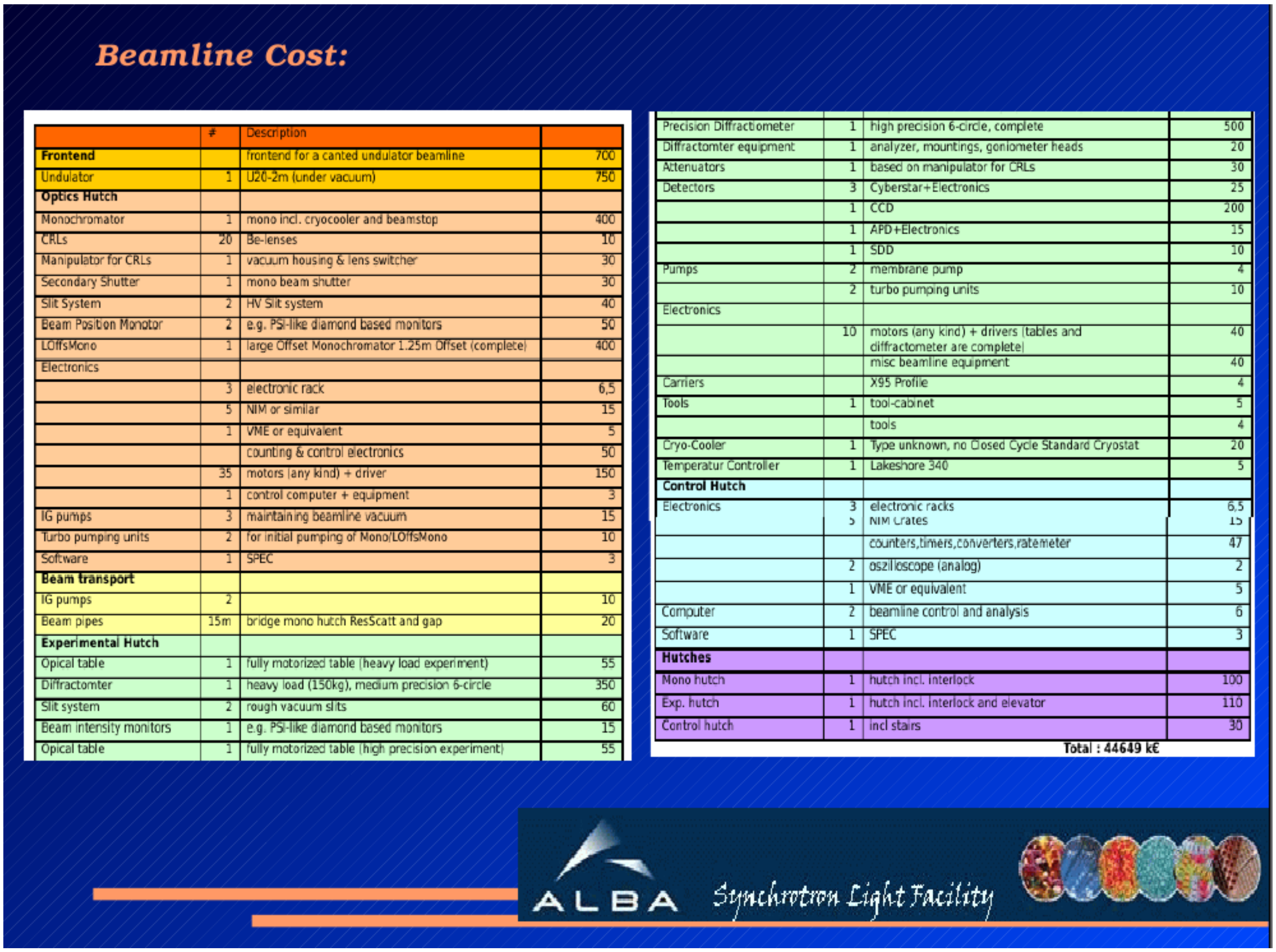


Figure: Parameters of the x-ray beam at the sample position using the µ-mode at HighRes. Top left the intensity in counts per second. Top right the contamination due to higher harmonic photons in counts per seconds. Bottom left the beam size in µm (FWHM), bottom center the divergence in µrad (FMHW) and bottom right the energy resolution in eV.

NOTE: All the presented graphics are approximated because we don't have the exact machine-source parameters, but the relationship of parameter between modes should be corrects.

2. The beamline cost.

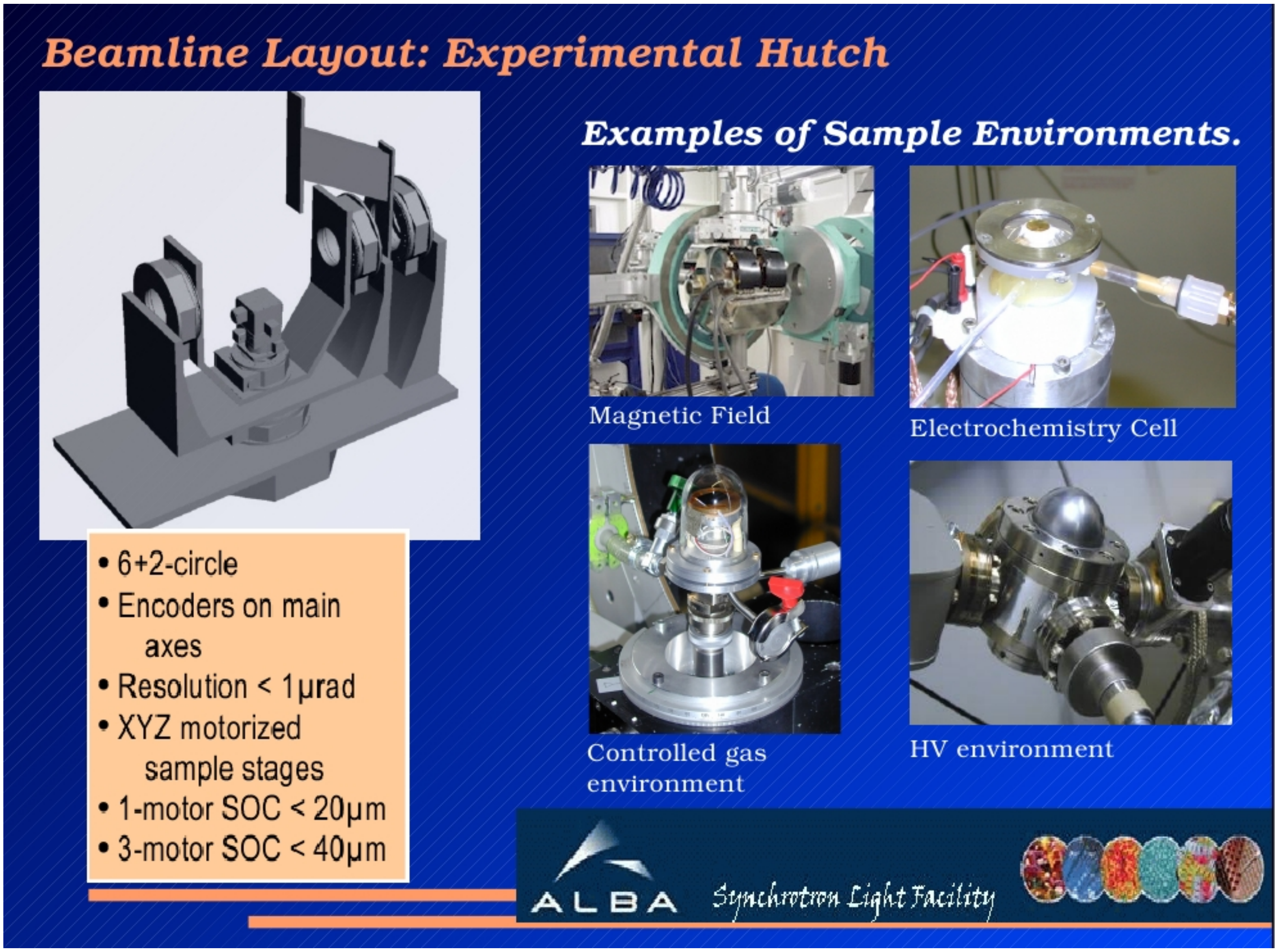
In the estimated beamline cost, presented at the SAC, there is an error in the total cost in an order of magnitude. The total resulting cost is 4465 k€. As it can be deduced from the optical configuration the proposed beamline has only one experimental hutch with only one end-station. This is the reason because it is not duplicated in the cost estimation.



	#	Description	
Frontend		frontend for a canted undulator beamline	700
Undulator	1	U20-2m (under vacuum)	750
Optics Hutch			
Monochromator	1	mono incl. cryocooler and beamstop	400
CRLs	20	Be-lenses	10
Manipulator for CRLs	1	vacuum housing & lens switcher	30
Secondary Shutter	1	mono beam shutter	30
Slit System	2	HV Slit system	40
Beam Position Monotor	2	e.g. PSI-like diamond based monitors	50
LOffsMono	1	large Offset Monochromator 1.25m Offset (complete)	400
Electronics			
	3	electronic rack	6,5
	5	NIM or similar	15
	1	VME or equivalent	5
		counting & control electronics	50
	35	motors (any kind) + driver	150
	1	control computer + equipment	3
IG pumps	3	maintaining beamline vacuum	15
Turbo pumping units	2	for initial pumping of Mono/LOffsMono	10
Software	1	SPEC	3
Beam transport			
IG pumps	2		10
Beam pipes	15m	bridge mono hutch ResScatt and gap	20
Experimental Hutch			
Opical table	1	fully motorized table (heavy load experiment)	55
Diffractomter	1	heavy load (150kg), medium precision 6-circle	350
Slit system	2	rough vacuum slits	60
Beam intensity monitors	1	e.g. PSI-like diamond based monitors	15
Opical table	1	fully motorized table (high precision experiment)	55
Precision Diffractiometer	1	high precision 6-circle, complete	500
Diffractomter equipment	1	analyzer, mountings, goniometer heads	20
Attenuators	1	based on manipulator for CRLs	30
Detectors	3	Cyberstar+Electronics	25
	1	CCD	200
	1	APD+Electronics	15
	1	SDD	10
Pumps	2	membrane pump	4
	2	turbo pumping units	10
Electronics			
	10	motors (any kind) + drivers (tables and diffractometer are complete)	40
		misc beamline equipment	40
Carriers		X95 Profile	4
Tools	1	tool-cabinet	5
		tools	4
Cryo-Cooler	1	Type unknown, no Closed Cycle Standard Cryostat	20
Temperatur Controller	1	Lakeshore 340	5
Control Hutch			
Electronics	3	electronic racks	6,5
	5	NIM Crates	15
		counters,timers,converters,ratemeter	47
	2	oszilloscope (analog)	2
	1	VME or equivalent	5
Computer	2	beamline control and analysis	6
Software	1	SPEC	3
Hutches			
Mono hutch	1	hutch incl. interlock	100
Exp. hutch	1	hutch incl. interlock and elevator	110
Control hutch	1	incl stairs	30

Total : 44649 k€

Relative to the cost estimation for the proposed samples environments, it has been considered to be provided most of them by users. In any case, the beamline can provided (as shown in figure) baby UHV chamber (not big ones like the UHV chamber at BM25, because they are already available at other facilities), electrochemistry cells, or gas controlled chamber. The estimated total costs is limited to 50 k€.



3. The proposed beamline in the European context.

The number of beamlines dedicated to surface x-ray diffraction in europe has been reduced in the last time. Some of the existing beamlines exhibits some limitations for the proposed scientific cases for this beamline:

I811 at Maxlab: It is a very simple configuration beamline, but due to its low backgound noise shows very good performance for organic self-assembled systems. The limitation is that it is dedicated only in a 15% of its beamtime for surface and 85% to EXAFS.

Material Science Beamline at SLS: This beamline has a very good resolution but the only available 2D detection configuration makes it very well adapted for high-scattering power surfaces and an almost perfectly arranged surfaces. For self-assembled organic monolayers the signal to background ration of the 2D detector is almost negligible.

The High-Resoltion beamline at PETRA: The configuration of this beamline is almost identical to our proposal for ALBA. However, given the outgoing beam characteristic of PETRA, even with the large offset monochromator the monochromatized beam is placed too close to the floor level. That makes that the available space for the sample environment is only of 5-6 cm. This is a huge limitation for the samples environments, even for UHV baby chambers.

BM25 at the ESRF: The high beamline divergence, induce so broad Bragg peaks that make almost impossible to reduce the structure of organic surfaces, overall, considering the large lattice units characteristics of such systems. The background noise is also much higher than the statistical noise.

Thus, only the surface dedicated beamlines at the ESRF (ID01, ID03 and ID32) can be competitors of the proposed beamline. These three beamlines cover the scientific range of the proposed beamline in only one.

The surface diffraction at Diamond we have no news about their technicals characteristics.