Design of mirror focusing system for the P23 nanodiffraction beamline at PETRA III extension

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Abstract

In this report, I describe the development of the mirror based focusing optics which will be used in P23 beamline PETRA III synchrotron.

Here, different configurations of elliptical and parabolic mirrors are studied with the aim to satisfy the requirements for the beamline, achieving a beam size in the micron range with divergencies which are in the order of ∼0.1 mrad. Finally, I briefly investigated the influence of the surface roughness of the mirrors on the quality of the focused beam. Besides, recommendations on the choice of optimal undulators parameters were made.

The modeling was done with montecarlo based raytracing software.

Contents

1 Introduction

Light is a powerfull tool for many disciplines in experimental science. In physics, chemistry, biology or even in medicine the light is frecuently used as a probe to obtain information from the samples to study. Light interacts with matter in several ways, which can be summarized in absorption, diffraction and reflection. From these interactions we can develop different experiments (spectroscopies, microscopies, diffraction...) where we can analyze the structure and properties of matter.

In this sense, synchrotrons have been shown to have an exceptional performance as light sources, leading to important and relevant scientificl results. Nowadays there are more than 50 synchrotrons around the world, serving scientist from many different nationalities and scientific areas.

The development of Synchrotron Radiation (SR) centers has boosted the previous mentioned experiments due to the SR characteristics. In the first place, synchrotron light covers a wide spectral range which goes from the infrarred to the hard X-ray wavelengths with a continuous spectrum, there is no other conventional light source which covers such a wide spectrum. But on practical purposes, synchrotron light is normally used from the far UV to X-ray, since for less energetic wavelengths there are conventional light sources of high quality, such as lasers.

Secondly, the flux is many orders of magnitude higher than that emitted by classical sources, which allows to perform real-time experiments in short intervals of time, with a very good signal/noise rate and with high resolution in energies. In the third place, the SR sources (specially undulators) have very small divergencies in both horizontal and vertical directions, which allows to maintain the beam with a size smaller than 1 mm^2 in distances of tens of meters.

All these characteristics explain why the concerned fields of research are so numerous, from biology (viruses or macromolecules...), to soft condensed matter (polymers, vesicles...) or material science (aggregates, precipitates...), the studied samples being liquids, gels or solids.

The aim of this report, which corresponds to my work developed during the DESY Summer Student Programme 2013, is to study the X-ray optics that can be implemented in P23 nano-diffraction beamline, which belongs to the PETRA III extension project. The main focus of the beamline is made on application of in situ and in operando diffraction techniques for investigation fundamental and applied research in physics and chemistry of low-dimensional and nanoscale systems. The research will focus both on the structure of objects and on processes in them, including chemical processes and behavior under non-ambient conditions, i.e. high pressure, low temperature, electrical and magnetic fields, laser irradiation.

During the programme, I have studied the characteristics of the different possible undulators that can be implemented in the beamline, and simulated a possible set up for the focusing optics of this beamline, based on the properties of the parabolic mirrors.

2 Simulation software

For the development of this project, I have used different software in order to study the emission of the undulator, the shape of the beam produced by it and to simulate the trajectory of the X-ray beam in the focusing system of mirrors.

In order to compare the performance of the different undulators and be able to chose the most adequate one, I have used SPECTRA 9.0 [1].

To study the shape and size, as well as the divergencies of the photon beam in the mirrors system, the ray tracing software SHADOW 2.3 [2] and the recently developed Python's package xrt [3], based on montecarlo simulation, have been used.

3 Results and discussion

3.1 Undulators

In the first place, we will study the beam generated by the two potential undulators available for the beamline: one with periodicity of 3,14 cm between magnets (which we will call Und1), and the other one with periodicity of 2,9 cm between magnets (which will be named Und2).

For the experiments that will take place in the beamline, we want to tune the energy of the source in a range from 8 to 25 eV in a continuous way by using the different harmonics of the emission produced by the undulator source.

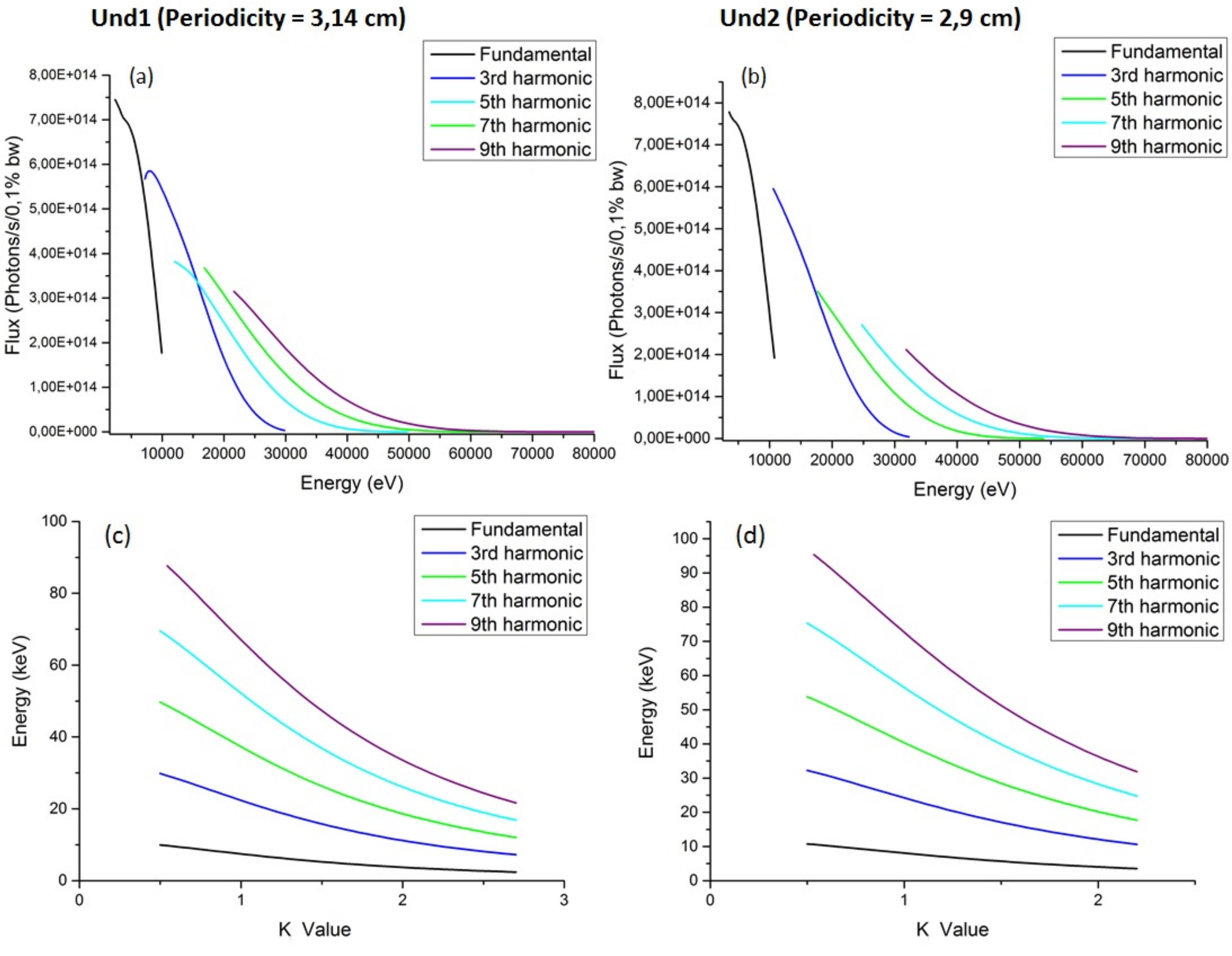

Figure 1: Photon flux for the different harmonics at 48m from the source for an undulator with periodicity of 2,9 cm between magnets in (a), and for periodicity of 3,14 cm between magnets in (b). In (c) and (d) the energy that each harmonic can achieve by tuning the parameter K is shown.

The results of the SPECTRA calculations for the photon flux at 48m from the undulator are shown in **Figure 1 a-d**. As it can be seen, Und2 can achieve higher energies by using a lower undulator parameter K (that is, by using lower magnetic fields, since K = $\frac{eB\lambda_u}{2\pi\beta m_e c}$ [4]), but it doesn't show a good overlap between the fundamental and the third harmonic in the energy regime around 10 keV, while Und1 shows a better overlap between the different harmonics, making possible to maintain the photon flux more stable when varying the energy of the light used.

This undulator has a gap value of 9,5, and uses a magnetic field B = 0,9209 T. It's periodic length is 3,14 cm and has a total length of 2m, that means 63 periods. It can achieve a maximun K value of 2,7, and a peak energy of the 1st harmonic at 2406,84 eV. The dimensions of the photon beam obtained from this source are shown in the table below.

	X	Z
Beam dimensions	141,4 μm	5,657 μm
Angular divergencies	7,071 μrad	1,768 μrad

Table 1. Size and divergences of the photon beam.

Being Y the propagation direction of the beam, Z the component perpendicular to the electron beam plane and X the perpendicular to both Y and Z.

3.2 Shape of the beam

Once selected Und2 as the best undulator for our purposes, we will study the characteristics of the beam emitted by it.

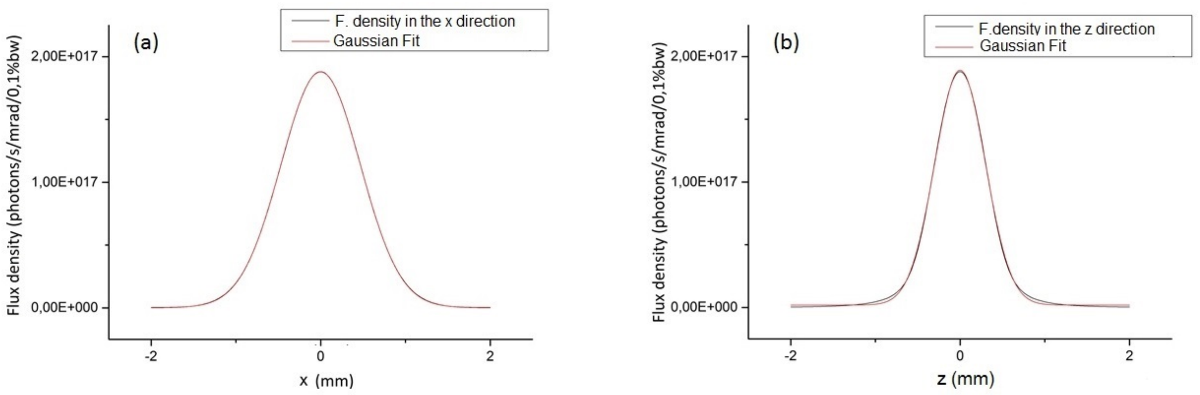

Figure 2: Flux density of the beam at 7243 eV and its gaussian fitting in **(a)** the x dimension and **(b)** the z dimension.

By using SPECTRA, we can get the cross section of the beam for different energies.In this case, we have characterized the emission of the 3rd harmonic of the undulator around its maximun of emission, in a range varying from 7208 to 7278 eV.

From these calculations, we can conclude that, from ∼7220 eV, the beam has approximately a gaussian shape, being the best situation around 7250 eV. It can be seen that the gaussian fitting and the calculated cross section match almost perfectly for both the x and z directions (**Figure 2(a)** and **(b)** respectively). This means that, for the ray tracing calculations, we can just take our source as a gaussian one, what makes the calculations easier and faster and should lead to a good agreement in the results when using different programs for ray tracing.

3.3 Optics of the system

Since we have selected the most appropriate undulator for generating our photon beam, and we have studied the shape of the beam produced, we want to build the optics for focusing the system.

In the projected beamline, diffraction experiments will take place. Along with spatial resolution, diffraction methods require a limited beam divergence, at least in the scattering plane. The divergence can range from seconds of arc for local strain or anomalous diffraction measurement in single crystals, for instance in bulk substrates with fine lateral structures, to fractions of degree for scattering on nanometer large objects. One can define several standard beam configurations that will be required at the beamline:

- highly collimated beam with a cross-section ~0.5x0.5 mm^2
- highly collimated beam with a cross-section ~0.05x0.5 mm^2 or ~0.5x0.05 mm^2
- moderately collimated beams with a cross-section ~10x10 μm^2
- a beam with low collimation and a cross-section under 1x1 μm^2, in extreme cases down to ~100x100 nm^2

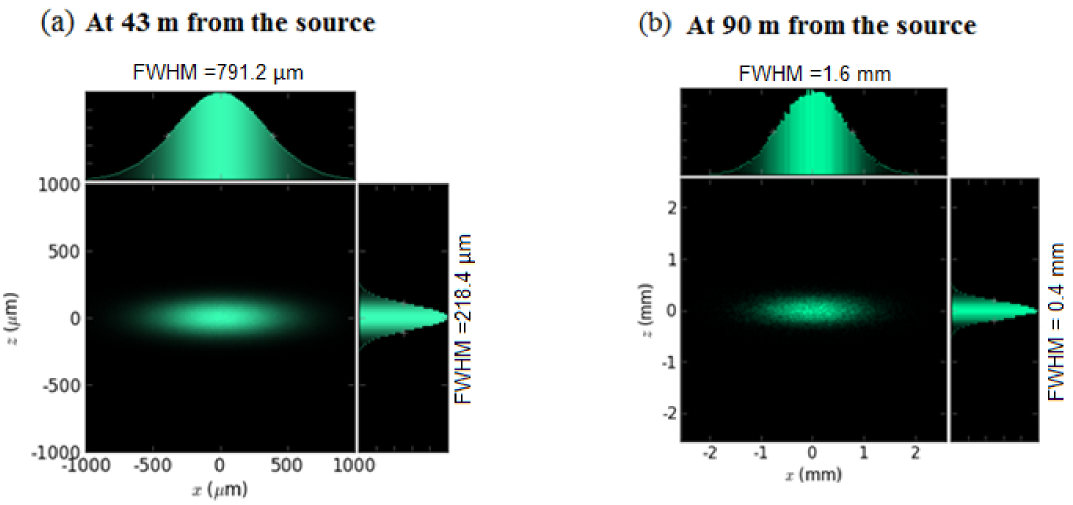

Figure 3: Cross-section of the beam at **(a)** 43m from the source and **(b)** 90m from the source.

The flexibility required in both the size and the shape of the beam, together with the spread of the beam in both the X and Z directions make necessary the development of a focusing optics which allows us to select the beam size and divergencies (the size of the focal spot in the two experimental hutches in the beamline when there is no focusing, shown in **Figure 3 (a)** and **(b)**, is larger than the experimental requirements).

In order to obtain such flexibility and wide range in sizes of the beam and maintain a collimated beam, we will take advantage of the properties of different geometrical shapes. In the first place, we will use an elliptical mirror, which focuses the beam into a point, creating a "point source" which will be collimated and focused by using parabolical mirrors. For all the situations studied in this report, the incidence angle of the beam with respect to the normal of the mirrors is of 89,8^o, and the energy spectrum of the source is taken as a single line of 7 keV.

3.3.1 Three mirrors system: elliptical + 2 paraboloid

With these elements, the simplest setup we can have is a three mirrors system with a first elliptical mirror and two parabolic ones. The first parabolic mirror will collimate the beam, so it can travel along the beamline, while the second will focus the beam to the source. As it can be seen in **Figure 4**, with this setup we get a beam with a Full Width at Half Maximun (FWHM) of 8.2 x 0.49 μm^2 and divergences as small as 0.6 x 0.1 mrad^2 at ∼90m from the source. But this system has several inconvenients, since it doesn't allow us to tune the ratio between the sizes in the X and Z direction independently (in some cases we would like to have a beam size with a cross-section much larger in one of the dimensions than in the other).

Furthermore, there are no suitable mirrors available to build this system, since the polishing techniques for these kind of mirrors are not very well developed. Thus, it is better to use cylindrical-shaped mirrors. Cylindrical-shaped mirrors take its name since they are created from geometrical shapes (such as a circle, parabola or ellipse) by the same mechanism than when creating a cylinder from a circle, so they act as plane mirrors in one dimension of the beam, and like geometrical mirrors in the other.

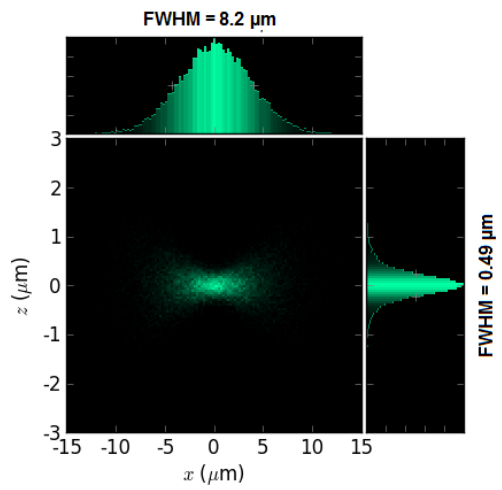

Figure 4: Cross-section of the beam after the system of 3 mirrors: a purely elliptical one which focuses the original gaussian beam, and two purely parabolic mirrors (one collimating and one focusing).

3.3.2 Independent focusing for X and Z dimensions: 3 mirrors + 3 mirrors

The best solution for this problem is to build two of this three mirrors systems, one for each dimension, so we can focus both the X and Z sides of the beam independently. By using this setup, we get with SHADOW a cross section with a FWHM of 2,22 x 0,1 μm^2 and the FWHM in the divergences is 2.0 x 0,56 mrad^2. This system gives good results in the vertical dimension Z, but the divergence is too big in the horizontal dimension for our purposes.

3.3.3 Independent focusing for X and Z dimensions: inserting a "condensor"

With the aim of improving the cross-section of the beam in the X dimension, we can add another two parabolic mirrors, which colimate and focus the beam again, acting as a "condensor" of the beam in this dimension. The ratio of the focal distances of the different parabolic mirrors has the capability of reduce the size of the beam the second time we collimate it, what gives the possibility of reducing the size of the beam maintaining a small divergence, as schematized in **Figure 5**. We can see that the dimension of the collimated beam will be reduced according to the ratio of the focal distances of the two parabolic mirrors according to the expresion:

$$I_2 = I_1 \tfrac{f_2}{f_1} \qquad (1).$$

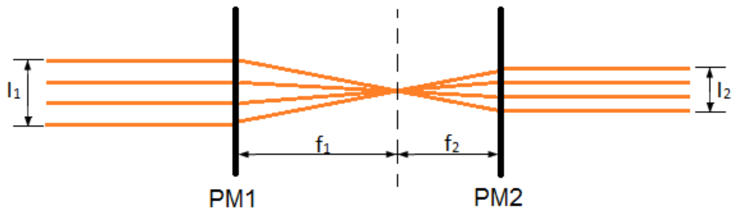

Figure 5: Scheme of the two parabolic mirror condenser used for reducing the beam size in the horizontal direction.

By including this set of two more mirrors, we get to reduce the size of the collimated beam in the X axis by a factor of 1/10. This gives a small beam which can travel along the beamline with very little dispersion in size and can be focused wherever we want.

In **Figure 6** we see that with a system of 6 mirrors (1 elipsoidal and 1 parabolic mirror placed horizontally and 1 elipsoidal and 3 parabolic placed vertically) we have achieved a beam cross-section at the source with FWHM of 0.21 x 0.15 mm^2, which means it has similar FWHM in both dimensions (the initial source was ~20 times bigger in the X dimension). The divergencies of this beam are as small as 67.3 x 0.365 μrad^2. After inserting another mirror focusing in the X direction, we can get a beam of $\sim 8\mu m$ with a divergence of 0.6 mrad in this direction.

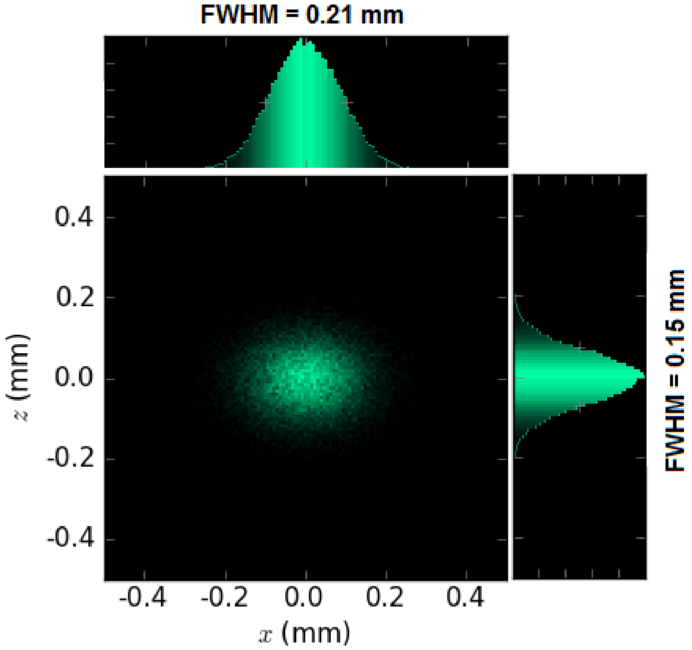

Figure 6: Cross- section of the collimated beam at ∼90m from the source after having been reflected by 6 mirrors: an elipsoidal and a parabolic mirror placed horizontally (collimating the Z direction) and an elipsoidal and three paraboic vertical mirrors (collimating the X dimension).

3.4 Surface roughness

Until now, we have seen different situations and studied how the x-ray beam behaves when interacting with the focusing optics developed. However, the imperfections of the focusing elements have not been taken into account. The wavefront error of the focused beam distorts the shape of the intensity profile on the focal plane and spreads the beam. The short wavelength of X-rays demands unprecedent accuracy in the manufacturing of the optical components to form an ideal spherical wave, so it's necessary to make an idea of how the roughness affects the optics of the system. In the best cases, the focusing of the hard x-ray beam can even break the 10 nm barrier [5].

Surface error (ripple Ampl/ripple Wavel)						Final spot size					# of lost rays
1st mirror	2nd mirror	3rd mirror	4th mirror	5th mirror		X(cm)	Y(cm)	X'(rad)	Y'(rad)		
0	0	0	0	0		0,0385	0,00403	4,16E-06	**0,000133**		821
2E-6/1	2E-6/1	2E-6/1	2E-6/1	2E-6/1		0,03923	0,00507	4,35E-06	**0,0016**		28895
2E-6/0,1	2E-6/1	2E-6/1	2E-6/1	2E-6/1		0,0426	0,00446	5,44E-06	0,00178		48189
2E-6/10	2E-6/10	2E-6/1	2E-6/1	2E-6/1		0,0379	0,00463	4,17E-06	0,00155		**18702**
2E-6/1	**2E-6/0,1**	2E-6/1	2E-6/1	2E-6/1		0,04145	0,0053	5,40E-06	0,00182		47353
2E-6/1	**2E-6/10**	2E-6/1	2E-6/1	2E-6/1		0,0385	0,00462	4,15E-06	0,00186		29875
2E-6/1	2E-6/1	**2E-6/0,1**	2E-6/1	2E-6/1		0,0379	0,00968	6,40E-06	0,018		44888
2E-6/1	2E-6/1	**2E-6/10**	2E-6/1	2E-6/1		0,0387	0,0041	4,31E-06	0,00149		27298
2E-6/1	2E-6/1	2E-6/1	**2E-6/0,1**	2E-6/1		0,0398	0,00516	7,00E-06	0,00147		30450
2E-6/1	2E-6/1	2E-6/1	**2E-6/10**	2E-6/1		0,0394	0,005	4,33E-06	0,00156		28971
2E-6/1	2E-6/1	2E-6/1	2E-6/1	**2E-6/0,1**		0,0394	0,00842	6,89E-06	0,00156		28895
2E-6/1	2E-6/1	2E-6/1	2E-6/1	**2E-6/10**		0,0392	0,005	4,32E-06	0,00161		28896
Best parameters											
2E-6/10	**2E-6/10**	2E-6/1	2E-6/1	2E-6/1		0,03845	0,00654	4,19E-06	0,00123		1542

Table 2. Dependance of the number of rays lost in the system of 5 vertical mirrors with respect to the surface roughness of the different components.

In our case, a study of the dependance of the cross-section of the beam at the sample with respect to the roughness of the mirrors reveals that the most critical mirror is the first eliptical one. In **Table 2** we can see that it is not necessary that the last mirrors have a great polishment quality, since changing the roughness doesn't increase the amount of rays lost significantly. On the other hand, the surface quality of the first one is critical. This behaviour is not the common one, in which normally the last mirrors are the ones which affect mostly the final spot. We can point to the parabolic shape of the mirrors used as a responsible of this situantion, since parabolic mirrors are free of some aberrations, like the spherical ones.

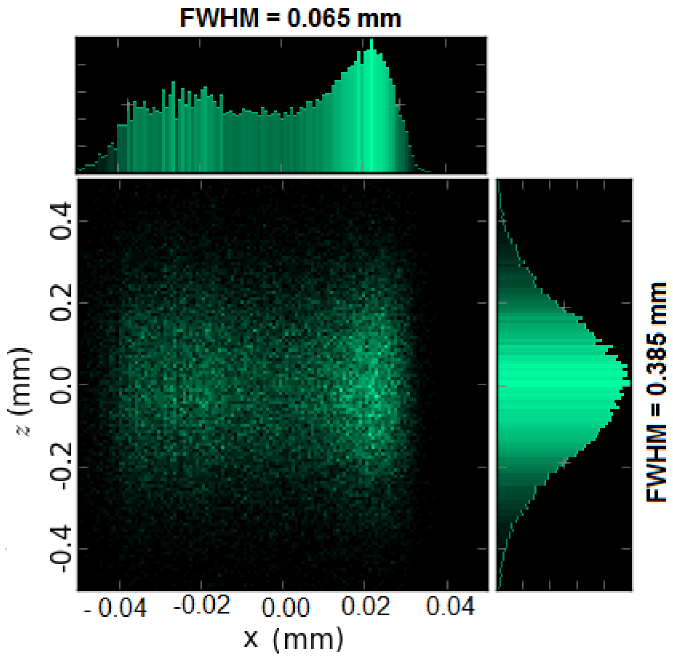

Figure 7: Beam cross-section when considering 5 vertical mirrors (focusing in the horizontal plane) with surface roughness.

The final spot after 5 mirrors focusing in the horizontal plane when considering roughness with the best parameters from **Table 2** is shown in **Figure 7**. We can see that the divergences are increased when considering roughness, and the original gaussian shape of the beam is lost.

4 Comments on the ray tracing simulating software

During the development of the project, some errors in the simulation software when using parabolic mirrors have been detected:

In SHADOW ray tracing software, it is said in the manuals that we must set the focus location at the source when we want the mirror to collimate the beam, and at the sample when we want it to focus the incident beam. However, to get the correct behaviour of the mirror, the selection has to be done in the opposite way. This error in the program is easily checked when simulating situations which have a solution known before hand: e.g we must select the focus location at the source for focusing an incident plane wavefront into a point, and we must select it at the sample for making a plane wavefront from a point source, just the opposite of how it should be.

In the case of xrt python package, the raycing modulus shows some problems when using the parabolic mirrors, showing results which dont match SHADOW's ones. Concretely, xrt shows a lost of the gaussian shape in a range at a certain distance of the mirror, and recovers the gaussian shape afterwards.

Furthermore, the symmetric shape of the incident gaussian beam is also lost. The evolution of the cross-section of the beam given by the xrt software after two vertical mirrors (an ellipsoidal focusing one and a paraboloidal collimating one) in which we would expect the beam to travel without modifying its shape, is shown in **Figure 8**.

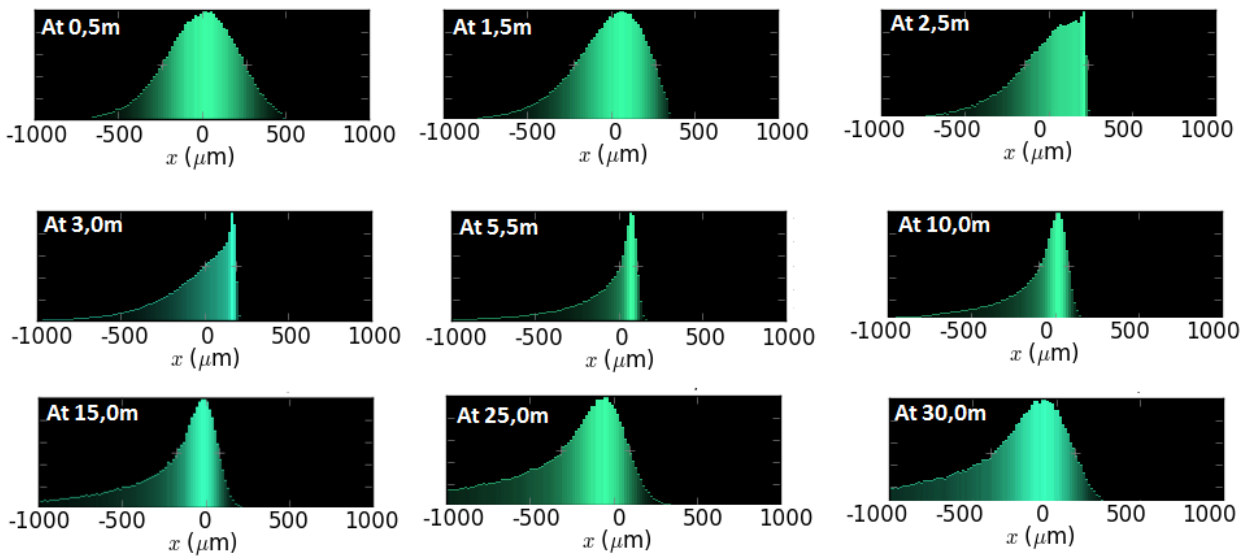

Figure 8: Profile of the cross-section of the beam in the horizontal axis obtained with xrt after the system of 2 mirrors: an elliptical and a parabolic one. The different plots show the evolution of the cross-section with the distance from the collimating parabolic mirror.

5 Conclusion

In this work, several simulations have been performed. Firstly, the tunning curves and characteristics of two different undulators have been studied, leading to the conclusion that an undulator with 3,14 cm of magnet periodicity gives a better covering of the whole range of energies which is interesting for the future beamline. Furthermore, it was shown that for a certain range of energies, the beam produced by this undulator has a gaussian cross-section, which improves and simplifies the simulation of the optical focusing of the system.

In the next step, a system of mirrors that can be implemented in the beamline has been simulated with both SHADOW and xrt Python package. From this simulations, we see that a system with 3 horizontal mirrors focusing the beam in the vertical direction and a system of 5 vertically placed mirrors focusing the beam in the horizontal direction leads to a wavefront with small size and divergencies, which can travel long distances without spreading and can be used in the two experimental hutches in the beamline.

The software developed can be easily used to study different situations of interest, the capability of separating the optical focusing in the two dimensions makes possible to have a wide range of beam sizes and shapes. For example, it will be easy with this kind of optics to get a "blade beam", very focused in one direction and spread in the other one, which is of interest in some experiments related to surface scattering. In the projected beamline, the last focusing mirror will be bimorph, so it can be deformed, giving flexibility in achieving a wide range of focal spot sizes. Besides, the insertion of a condenser of two parabolic mirrors leads to such a small and collimated beam that can be used to achieve intermediate focal spots, without the necessity of having the last focusing mirror.

Finally, we have briefly characterized the effect of different surface roughness in the mirrors. In our case, the most critical mirror (that is, the one which quality should be the best) is the first ellipsoidal one, not playing the roughness an important role in the last parabolic ones. As an additional point, this project has given a better understanding of the ray tracing software used (SHADOW and xrt), and has checked their performance, leading to the detection of some problems in those programs.

References

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