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Simulation and optimization of the SIRIUS IPE soft X-ray beamline

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ABSTRACT

The soft X-ray beamline IPE is one of the first phase SIRIUS beamlines at the LNLS, Brazil. Divided into two branches, IPE is designed to perform ambient pressure X-ray photo-electron spectroscopy (AP-XPS) and high resolution resonant inelastic X-ray scattering (RIXS) for samples in operando/environmental conditions inside cells and liquid jets. The aim is to maximize the photon flux in the energy range 200-1400 eV generated by an elliptically polarizing undulator source (EPU) and focus it to a 1 μ m vertical spot size at the RIXS station and 10 μ m at the AP-XPS station. In order to achieve the required resolving power (40.000 at 930 eV) for RIXS both the dispersion properties of the plane grating monochromator (PGM) and the thermal deformation of the optical elements need special attention. The grating parameters were optimized with the REFLEC code to maximize the efficiency at the required resolution. Thermal deformation of the PGM plane mirror limits the possible range of c_{ff} parameters depending of the optical concept and the simulations of the IPE beamline. We compare simulations performed by geometrical ray-tracing (SHADOW) and wave front propagation (SRW) and show that wave front diffraction effects (apertures, optical surface error profiles) has a small effect on the beam spot size and shape.

Keywords: soft X-ray beamline, ray-tracing, wave front propagation, grating efficiency

1. INTRODUCTION

The high brilliance of 4th generation sources enabled the improvement and spread of X-ray emission spectroscopies, due to the photon hungry process and the high demand for spectral resolution. The IPE beamline, coupled with the high brilliance of the new Brazilian synchrotron radiation source – SIRIUS, has been designed to provide access for a large community to state-of-the-art soft X-ray characterization techniques, being capable of in situ investigation of materials under different environments and conditions. This modern concept allows the study of structure-function correlations, which is fundamental for better understanding and improvement of materials in several applications like catalysis and energy storage devices. The beamline will serve two end stations dedicated to Ambient Pressure X-ray Photo-electron spectroscopy (AP-XPS) and Resonant Inelastic X-ray Scattering (RIXS).

Resonant inelastic X-ray scattering is a second order optical process with very low cross section demanding high intensity incident radiation and efficient detection of scattered photons. At the same time, very high resolution is necessary to separate the spectral features that carries information about different electronic and vibrational excitations in the materials. Hence, optimizing the transmission of the monochromator at a target resolution is crucial to enhance the scientific throughput of the beamline and improve the statistical quality of the data. The great challenge for the RIXS end station is the vertical spot size at the sample, which must be less than 1 μ m for allowing slit-less operation. Smaller beam spot allows better resolving power and reduces the spectrometer arm length. The beamline must be optimized to provide the highest transmission possible for the target energy resolution of 15 meV at 930 eV, which combined with the RIXS spectrometer, will provide resolution in the order of 20 meV.

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Advances in Computational Methods for X-Ray Optics IV, edited by Oleg Chubar, Kawal Sawhney, Proc. of SPIE Vol. 10388, 103880D · © 2017 SPIE CCC code: 0277-786X/17/\$18 · doi: 10.1117/12.2273971 Therefore, we used the numerical code REFLEC¹ to maximize the monochromator efficiency. For the energy resolution of the monochromator, we used the new interface for SHADOW kernel, ShadowOui². A great advantage of this tool is that it provides a python script for a beamline setup, which can be used to automate parameters inputting, scanning and data analysis. Also, we show that the partial coherence of the source affects the beam focusing at the exit slit and consequently wave propagation simulations with the Synchrotron Radiation Workshop (SRW³) are essential for accurate performance determination. We intend to show that a detailed optical design depends on many simulation tools.

2. UNDULATOR PHOTON SOURCE

The source of the IPE beamline, operating in the energy range of 200 eV and 1400 eV, requires full polarization control with photon flux in the order of 10¹⁴ Ph/s/100mA/0.1%bw. A 3.6 m long DELTA undulator with 52.5 mm period fulfils those requirements. The DELTA undulator, originally developed by Cornell University⁴ and further improved by LCLS⁵, is an elliptical polarized undulator (EPU) and consists of four quadrants of permanent magnet blocks moving longitudinally at fixed gap. Sliding opposing quadrants controls the K-value and sliding the quadrant pairs relative to each other the phase and polarization. The fixed and small gap allows a more compact design and higher magnetic fields (lower energies) compared to conventional APPLE type EPU's. We are developing a DELTA undulator in-house in collaboration with the Brazilian company WEG⁶.

Table 1. Storage ring and Delta undulator parameters. The beam size and divergence are for the low- β straight section.

Storage ring		Delta undulator	
Energy	3.0 GeV	Period Length	52.5 mm
Electron beam current	350 mA	Total Length	3.6 m
Emittance (no IDs)	0.251 nm.rad	Max. K-value (linear)	5.85
Electron beam size (r.m.s)	18.7 (h) x 1.9 (v) μ m ²	Max. K-value (circular)	4.14
Electron beam divergence (r.m.s)	12.7 (h) x 1.2 (v) urad ²		



Figure 1. Photon beam size (left) and divergence (right) with DELTA undulator source.

In the soft X-ray range, the beam size and divergence of the photon source is strongly energy dependent and with fourthgeneration synchrotron as SIRIUS strongly affected by the energy spread effect of the electron beam. In the ray-tracing code SHADOW we use the geometrical (Gaussian) source. Source size and divergence are calculated analytically as proposed by Tanaka & Kitamura⁷. This approach, valid for undulator radiation considers simultaneously the finite emittance and the energy spread of the electron beam in the storage ring. The Synchrotron Radiation Workshop (SRW) software calculates accurately the emission over the undulator length based on the electron beam parameters and the magnetic field structure.

3. OPTICAL DESIGN

The optical design of the IPE beamline is based on the collimated PGM^8 (cPGM) design. Compared to the commonly variable line space grating design, it allows more flexibility in optimizing for high energy resolution, high photon flux or high spectral purity with the free choice of the c_{ff} parameter.

3.1. Beamline layout

The first optical element is a horizontal deflecting toroidal mirror (CM) located 27 m from the source collimating the beam vertically and focusing it horizontally into the exit slit. The PGM sitting 2 m downstream the CM consists of a plane mirror, to change the entrance angle of the grating, and interchangeable plane gratings with constant ruling. A sagittal cylindrical mirror (FM) focuses the vertically dispersed beam into the exit slit. A plane side deflecting mirror (DM) located 2 m downstream the FM deflects the beam to the AP-XPS branch, whereas without the DM the beam continues in the RIXS branch. An ellipsoidal mirror (RMR and RMX) focuses the beam to each experimental station.



Figure 2. IPE beamline optical layout.

3.2. PGM mechanical design

The guiding line for the mechanical design of the PGM considers that the grating and the plane mirror can be manufactured and measured. The grating optical active length amounts 140 mm is defined by accepting 4σ of the vertical beam over the energy range of 200 eV to 1600 eV and for c_{ff} -values below 5. The optimization of the offset value is a compromise between a reasonable length of the plane mirror and avoiding shadowing effects on the beam. Hence, we obtained an optimum offset of 18 mm. The rotation axis of the plane mirror is located on top of the drawing and of the plane grating in the gratings center. Based on the formulation described by Pimpale⁹ we obtained an RC = 27.3 mm between the PM and its center of rotation (Figure 3). Thus, the beam is moving along the PM depending on energy and c_{ff} settings.



Figure 3: Mechanical scheme of the PGM

3.3. Minimizing heat load effects on white beam optics

Synchrotron mirrors exposed to a white beam (high power load) deform into a convex shape. A cooling scheme commonly used to deal with the high heat load and reduce the thermal deformation is the indirect side cooling with water. However, the low emittance of SIRIUS and the large incidence angle (~1 degree) result in high power density absorbed on the mirror surface. This requires an internal cooling scheme. The silicon substrates of the toroidal mirror and the plane mirror have eight channels of 1 mm width and 1 mm spacing in between. The channels have a 5 mm height and are 1 mm distant from the reflecting surface. A water flow of 0.5 l/min through each channel corresponds to a convection coefficient of 20000 W/m²K. The plane grating absorbs a power density (projected) less than 0.04 W/mm² and therefore its cooling scheme is conventional side cooling. Temperature distribution and thermal slope were calculated by finite element analysis (FEA) code ANSYSTM. The power density absorbed on the mirror or grating is applied as surface heat flux in the FEA model. The total power generated by the DELTA undulator in horizontal polarization mode (largest power load) amounts 10 kW on the maximum k-value of 5.85 and 350 mA ring current. Based on the limitations in the mechanical design, especially the maximum length of the grating, we defined the horizontal acceptance to 140 µrad (higher than 4\sigma at energies > 200 eV). The vertical acceptance amounts 210 µrad (front-end aperture). Inside this aperture, the total incident power is 600 W.

OE	Total absorbed power [W]	Absorbed power density (normal incidence) [W/mm²]	Mirror incidence angle [°]	Mirror length [mm]	Operating conditions
Toroidal mirror	265	16.5	0.8	280	200 eV, 0.8°
Plane mirror (a)	116	5.4	9.0	450	Not operational, PM at maximum incidence angle
Plane mirror (b)	113	5.8	5.8	450	400 eV, $c_{\rm ff}$ =1.4
Plane grating	7	1.2	1.7	140	1000 eV, $c_{ff}=2.0$

Table 2: Power load, calculated by SPECTRA¹⁰ and OE parameters.

Table 3: FEA	results	for the	CM,	PM	and	grating.
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	Max. Temperature [K]	Local flatness [µrad]	2σ flatness [µrad]	Max. von-Mises stress [MPa]
Toroidal mirror	301.5	1.073	0.166	1.9
Plane mirror (a)	309.5	4.593	0.152	4.3
Plane mirror (b)	304.2	1.551	0.119	2.3
Plane grating	299.2	0.531	0.125	0.3

FEA was performed for the toroidal mirror, the plane PGM mirror and the plane PGM grating. The resulted surface height profile can be further used in ray-tracing and wave propagation simulation to characterize the influence of the deformation onto the beamline performance. The local flatness¹¹, defined as standard deviation of the slope inside the illuminated beam length, gives a good indication of this influence without running simulations. A local flatness value in the same order as the r.m.s. slope error from polishing does not change the performance. Nevertheless, we define the " 2σ flatness" as the r.m.s slope inside the footprint relative to only 2σ of the beam distribution, which better characterizes the heat load effects. This procedure eliminates the border effect, where the slope increases strongly along the borders of the illuminated areas. Since 2σ beam size includes almost 70% of the photon flux, the 2σ flatness is a better estimate on how the deformation affects the beam performance.

The toroidal mirror operates under fixed incidence angle and power load, and its r.m.s. slope error from polishing is specified to 250 nrad. In the extreme operational case (200 eV), its thermal deformation corresponds to a 2σ flatness of 166 nrad (Table 3, Figure 4). Despite the increase in total slope error, ray-tracing simulation including the thermal deformation of the toroidal mirror confirmed that there is no change on beam size and shape in focus. We also considered a case for the maximum magnetic field of the undulator (K = 5.85, E₁ = 90 eV). The 2σ flatness achieves 510 nrad, but still there is no significant influence, since the horizontal beam size also increases considerably (see Figure 1).



Figure 4. Toroidal mirror - Surface deformation (left) and respective slope profile (right) along meridional axis.

For the plane mirror, we performed the FEA for the worst operating condition related to the highest absorbed power density (400 eV, c_{ff} =1.4, case (b)). Assuming the polishing slope error and the 2 σ flatness add up quadratically, we obtain 155 nrad r.m.s. slope error. Up to this limit the vertical beam size and shape is not affected, as confirmed by ray-tracing simulations. Therefore, we specified the polishing slope error of the PM to 100 nrad r.m.s. The small dip in the center of the slope profile is caused by a symmetry artefact of the FEA.



Figure 5. Plane mirror (b) - Surface deformation (left) and respective slope profile (right) along meridional axis.

A second FEA simulation study for the PM considers an extreme incidence angle (case (a)), which is the mechanical limit of this rotation axis. This is not a situation for normal operation, but to verify if the mirror sustains the high absorbed power density. We obtained a maximum von-Mises stress of 4.3 MPa. A standard value to guarantee silicon performance is a limit stress of 7 MPa, noted as "rule of thumb" by Schwertz¹², which represents a probability of failure of approximately 1 in 42 million. The failure considers the appearance of micro-cracks in the silicon bulk material. The criterion is based on very conservative statistics. Hence, we do not expect permanent deformations or cracks in the plane mirror.

The plane grating absorbs only 7 W total power and the absorbed power density projected on the grating amounts 0.04 W/mm². Therefore, we use a conventional side cooling scheme on the grating. The resulted 125 nrad 2σ flatness is inside the expected limits compared to the polishing slope error (100 nrad).

3.4. Ray-tracing vs. wave propagation simulations

The achievable resolution at the experiment can be estimated by the vertical linear energy dispersion and the spot size at the exit slit. The beam intensity contribution from an energy ϵ with small deviation from a reference energy at vertical position ($y_0(\epsilon_0) = 0$), passing through a slit with opening ζ is given as:

$$I(\epsilon) = \int_{-\zeta/2}^{\zeta/2} \frac{e^{\frac{(y-y_0(\epsilon))}{2\sigma_y^2}}}{\sqrt{2\pi\sigma_y^2}} \, dy = \frac{1}{2} \left(\operatorname{Erf}\left[\frac{-2\epsilon + \frac{dE}{dy}\zeta}{2\sqrt{2} \frac{dE}{dy} \sigma_y} \right] + \operatorname{Erf}\left[\frac{-2\epsilon + \frac{dE}{dy}\zeta}{2\sqrt{2} \frac{dE}{dy} \sigma_y} \right] \right) \tag{1}$$

The vertical position of the energy ϵ is defined by $y_c(\epsilon) = \epsilon/(dE/dy)$ with the linear dispersion dE/dy. This leads to the energy deviation (r.m.s.) passing through the slit.

$$\Delta E = \sqrt{\langle \epsilon^2 \rangle} = \sqrt{\frac{\int \epsilon^2 I(\epsilon) \, d\epsilon}{\int I(\epsilon) \, d\epsilon \, d\epsilon}} = \frac{dE}{dy} \sigma_y \sqrt{1 + \frac{\zeta^2}{12\sigma_y^2}} \tag{2}$$

Hence, the maximum resolution at almost closed exit slit is simply given by the linear dispersion multiplied by the focal spot size (r.m.s.) at the experiment (RIXS). In our simulations, we use the resolution for the slit size $\zeta = 4\sigma_y$.

The grating efficiency was calculated by parametric execution of the REFLEC code (part of the RAY software package). Blazed profile is preferred compared to laminar profile because of its higher efficiency. We calculated the efficiency maps varying line density k_0 , blaze angle δ and c_{ff} -value. The efficiency is then multiplied by the reflectance of the plane mirror at respective incidence angles. The energy resolution at the exit slit position is calculated using equation (2) from the results of ray-tracing simulations with SHADOW. Repeating this procedure by scanning k_0 and c_{ff} -value, we obtain energy resolution maps. Combining the resolution maps with the efficiency maps (Figure 6), we find optimized values for k_0 and δ maximizing the total transmitted intensity of the PGM. The complete process was performed for different energies inside the operating range.



Figure 6: Energy resolution map (left) and effective efficiency map (right) with the optimized $k_0=1100$ lines/mm and $\delta=1.0^{\circ}$.

Figure imperfections on the grating surface cause beam broadening and this can spoil the energy resolution. Therefore, we need to consider surface figure errors of the grating in the SHADOW simulations. As an example, we show the resolution maps for 150 nrad and 300 nrad (r.m.s.) slope error. The required energy resolution of 15.3 meV at 930 eV can be achieved for instance with $k_0=1000 / c_{ff}>6$ or $k_0=1600 / c_{ff}>3$ using a grating with 150 nrad slope error and with $k_0=1400 / c_{ff}>8.5$ or $k_0=1800 / c_{ff}>4$ using a grating with 300 nrad slope error (Figure 7). Hence, a substrate with smaller slope error operates at higher efficiency with lower k_0 , which is easier to manufacture. The final grating parameters chosen were $k_0=1100$ lines/mm, $\delta=1^0$ and the polishing slope error < 100 nrad.



Figure 7: Energy resolution map in the (k_0 , c_{ff}) space, considering the Exit Slit aperture equal to $4\sigma_y$, for (left) 0.15 and (right) 0.3 µrad RMS slope error on the grating. The black points indicate the minimum c_{ff} value that achieves the requires resolution for each k_0 .

Horizontal and vertical beam distributions at exit slit position without slope errors calculated with ray-tracing and wave propagation simulation agrees very well. Including slope errors, the horizontal beam broadens less with SRW. In the vertical direction ray-tracing overestimates the beam broadening and intensity loss (Figure 8). The wave propagation shows small satellite features in vertical direction (considering slope error). The target resolution is achieved in the optimized condition, if the vertical beam size (2.35σ) is smaller than 16 µm, which is satisfied even considering both plane mirror and grating figure errors, in both software.



Figure 8: Horizontal (left) and vertical distribution of the beam at exit slit position, calculated by SRW and SHADOW without (ideal) with (non-ideal) considering slope errors.

Radiation emitted from the DELTA undulator is partially coherent due to the very low emittance of the SIRIUS storage ring. Focusing a partially coherent beam obeys wave optics rather than geometrical optics¹³. A parameter showing whether wave optics (Gaussian beams) behavior is relevant for the calculation of the exact focal distance is the Rayleigh length Z_R at the focal position, where σ is the beam size at focus point, λ the wavelength and ξ the coherence length¹⁴.

$$Z_R = \frac{\pi \sigma^2}{\lambda} \left[1 + \left(\frac{\sigma}{\xi}\right)^2 \right]^{-\frac{1}{2}}$$
(3)

If the beam waist σ and beam divergence σ' at the focus are known, Z_R can be estimated by $Z_R = \sigma/\sigma'$. Calculating Z_R at 930 eV using SRW propagation results in a value of 2.3 m in horizontal direction and 0.07 m in vertical direction. The image distance of an optical element in wave optics is defined as the global focusing equation¹⁵, where *p* is the source distance, *q* the image distance and *f* the focal distance. For $Z_R \ll f$, the global focusing equation converges into the thin lens equation, where the optical system is fully characterized by geometrical optics.

$$q = f + \frac{p - f}{\left(\frac{p}{f} - 1\right)^2 + \left(\frac{Z_R}{f}\right)^2}$$

$$\tag{4}$$

Applying the focusing conditions at the exit slit position to the global focusing equation, we observe that the image distance in horizontal plane changes significantly compared to the thin lens equation because of the large Z_R . By correcting the meridional radius of the toroidal mirror (CM) we can correct for this effect. The exact radius was determined by simulations with SRW, which considers the partial coherence of the beam accurately, as well as diffraction effects from beam clipping. Due to the energy dependence of Z_R the CM becomes a chromatic focusing element in the horizontal plane¹³. Based on the scientific cases, the IPE beamline is optimized for an energy of 930 eV. Therefore, the meridional radius of the CM was corrected for 930 eV. Simulations performed by SRW show a shift of

the horizontal focus (exit slit position) 0.2 m upstream for 1600 eV and 0.3 m downstream for 400 eV. The change of horizontal beam size caused by that shift after correction is below 1.5%.



Figure 9: Horizontal beam size along beam propagation axis near the nominal exit slit position of 58 m for 400 eV (blue dots), 930 eV (red dots) and 1600 eV (black dots) considering the focal distance given by geometrical optics. * shows the horizontal beam size with corrected radius of the CM for 930 eV (black triangles). The solid lines are linear regressions from the Gaussian beam propagation equation.

At the sample position, the numerical aperture is relatively large, and the beam size is dominated by the source demagnification. Thus, the focal position at the sample is highly predictable by geometrical optics (thin lens equation). This is confirmed by the simulations with SRW and SHADOW (Figure 10). Nevertheless, the beam is broader using ray-tracing, if we consider slope errors. The requirement for energy resolution, defined by the RIXS scientific case, is fulfilled if the vertical beam size at the sample is less than 1 μ m (2.35 σ) at 930 eV. In both ray-tracing and wave propagation, the beam size ranges from 1 μ m at 400 eV to 0.4 μ m at 1600 eV. The advantage of a single horizontal deflecting ellipsoidal mirror is that the figure errors from polishing do not affect the vertical distribution significantly. Ellipsoidal mirrors are extremely complex to manufacture with high quality, but the performance of the beam is not affected significantly, since the horizontal beam size is in the order of 3 μ m.



Figure 10: Horizontal (left) and vertical distribution of the beam at RIXS station, calculated by SRW and SHADOW without (ideal) with (non-ideal) considering slope errors.

4. CONCLUSION

We have shown a complete optical design process for a state-of-the art soft x-ray beamline dedicated to RIXS and XPS. The advent of 4th generation synchrotrons demand detailed simulations, where the partial coherence of the beam must be accounted for, which is generally not modeled in analytical calculations. In the IPE beamline, the optical system design showed that the beam properties, such as energy resolution and flux, are directly linked not only to the optical properties, but also to the mechanical and thermal aspects of the beamline. Due to these connections, we combined several simulation tools to try to model the beam performance as close as possible to real operation conditions.

Ray-tracing with proper source configuration provides good estimates of the beam properties, and its flexibility allows large parametric execution with little computational effort. However, geometrical optics is limited to the uncoherent condition, and cannot be used as the only simulation tool. SRW was used to define the precise mirrors specifications.

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