Use of astigmatic re-focusing at HP-XPS end-station

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Abstract. In this paper we present the refocusing optics for the new high pressure photoelectron spectroscopy (HP-XPS) branch line at MAX-lab, based on a plane grating monochromator with vertically collimated beam. For the HP-XPS instrument, the required spot size is dictated by the small geometric acceptance of the HP-XPS electron energy analyzer. Whereas a pair of bendable mirrors in a KB configuration has some advantages as refocusing elements, we have studied whether similar performance can be achieved with a single non-bendable mirror. In this solution, however, the need for strong horizontal magnification results in a strong vertical magnification and into a very asymmetric image, the height being just a fraction of the width. We have studied through an analytical geometrical model and ray tracing simulations the use of astigmatism to increase the vertical beam size up to the geometric acceptance of the detector. As a result the vertical beam size at sample plane is mostly determined by the photon angular distribution and is not dependent on the exit slit aperture size. In addition the vertical beam size can be controlled by the grating $c_{eff}$ parameter, making possible to adjust the photon density and minimize sample damage by the radiation.

1. Introduction

Within the next year, beamline I511 at the MAX II storage ring will be updated with a plane grating monochromator illuminated with a collimated beam [1], which will serve two branch lines. After the plane grating monochromator the beamline is split into two branches, one of them dedicated to Resonant Inelastic X-ray Scattering (RIXS) and the other to High Pressure Photoelectron Spectroscopy (HP-XPS). The main constraints to the geometry of the beamline are imposed by the RIXS branch, in which both a good energy resolution and a small vertical spot height are required.

The HP-XPS end-station described in Ref.[2] is equipped with a near ambient pressure electron spectrometer. To be able to operate at ambient pressure, a pre-stage of differential pumping is necessary between the analyzer and the sample environment. Towards the differential pumping system a small aperture limits the gas flow and different aperture sizes can be used to reach different maximum pressures. Presently, the smallest aperture applied here has a diameter of $300\mu m$, but can be replaced by even smaller apertures. This small aperture limits the maximum geometric acceptance of the spectrometer for the incoming electrons. To take full advantage of the incoming photons, the spot size in the sample plane must match this geometric acceptance. In the case of the $300\mu m$ aperture, an optimum detection efficiency is achieved with a photon spot size of about $100 \times 100\mu m^2$ at the sample.
The elevated pressure required at the sample is realised in a retractable high pressure cell with a X-ray window (Si\(_3\)N\(_4\) membrane), preserving the vacuum environment of the analysis chamber. In addition, a stage of differential pumping using a beam insulation ion pump\([3]\) is placed between the end station and the beamline, which allows measurements without the high pressure cell at pressures from UHV up to \(10^{-5}\)mbar. This makes possible an enhancement of the photon flux at these pressures due the absence of an X-ray window. Although the differential pumping makes the alignment harder, it implies that the entire pressure range from UHV to \(\approx 10^{-1}\)mbar is available for experiments at optimized conditions.

The available space at the MAX II ring limits somewhat the possibilities for the HP-XPS branch optics. The energy resolution requirements are not as stringent as for the RIXS branch, but the relatively wide source (830\(\mu\)m, FWHM)\([4]\) should be focused to ca. 90\(\mu\)m in size. The geometry used here, 54\(^\circ\) between the electron spectrometer and the photon beam (Fig. 1), results then in a horizontal beam size of about 150\(\mu\)m. For maximum transmission, an aperture with a diameter slightly larger than 300\(\mu\)m would be ideal. The beamline is designed with the possibility to be transferred to the new MAX IV facility \([5]\), and there the chosen geometry will produce an optimal spot size without any requirement for changing the optical elements in the beamline.

A conventional KB system has some advantages over a single mirror solution, namely an easy control of the beam position and of the spot size. However, a single mirror solution means less reflection losses, simpler alignment and in this particular case provides a horizontal beam to the experiment. Moreover, the toroidal mirror can also be used to control the beam position by adjusting the pitch and roll angles. This qualitative comparison motivated us to study whether a good performance can be achieved with a single non-bendable toroidal mirror.

For such a single mirror solution, the large horizontal source size requires a strong demagnification in the horizontal plane, which in turn results also in a strong vertical demagnification. The differential pumping necessary between the sample environment and the refocusing mirror limits the minimum distance between them to 1.5\(m\) and results in a vertical demagnification of 3:1, considering the 6\(m\) available between the sample and the exit slit. As a consequence, the image has a vertical dimension considerably smaller than the horizontal size at the sample plane, since a relatively small exit slit aperture is necessary to fulfill the energy resolution requirements.

In order to decrease the photon density and avoid sample damage by radiation, it is necessary to increase the vertical beam size up to the geometric limit dictated by the HP-XPS spectrometer acceptance. This is achieved using astigmatism simply by moving the nominal vertical focus further from the sample plane, while the nominal horizontal focus remains at that plane (Fig. 1). As a result the vertical beam size at the sample plane is determined mainly by the divergence of the beam at the image plane \((\sigma'_I)\), which in turn has a linear dependence on the source divergence and the so-called fix focus constant \(c_{ff}\) of the monochromator. A further advantage is that the vertical beam size at the sample plane will not depend on the slit aperture, as will be shown.

2. Geometric description of the astigmatic beam solution

We can use a simple geometric approach to estimate the vertical beam size at the sample position in case of an astigmatic focus. Here we assume that we have a point source and omit the imperfections of the optical elements.

The source distance \(\delta_{-M1}\) to the vertically collimating mirror (M1, see Fig. 1) together with the vertical source divergence \(\sigma'_I\) define the vertical extent of the beam, \(w_{M1}\), that reaches the grating: \(w_{M1} = \delta_{-M1} \cdot \sigma'_I\). This vertical beam size is then magnified by the projection over the surface of the plane grating in a well known manner \([6]\) by the fix focus constant \(c_{ff}\), and thus by the incident and diffracted angles of the grating. This results in a vertical beam size \(w_{PG}\)
Figure 1. Scheme of the HP-XPS branch at I511. M4 refocus the beam on the sample position in horizontal direction, whilst the vertical focus is separated by a distance \( \Delta \) (astigmatic focus).

After the plane grating of \( w_{PG} = w_{M1} \cdot c_{ff} \).

Assuming that the toroidal focusing mirror M3 focuses this beam onto the exit slit, we get a divergence \( \sigma'_{M3} \) after the focusing mirror. This is also the divergence of the incoming beam, \( \sigma'_{M4} \), at the last mirror M4 and is given by \( \sigma'_{M4} = \sigma'_{M3} = \frac{w_{PG}}{\delta_{M3-ex}} \), where \( \delta_{M3-ex} \) is the distance between the focusing mirror M3 and the exit slit. Finally, the divergence \( \sigma'_{I} \) at the image plane is given by the vertical magnification of the refocusing mirror M4 multiplied by the divergence \( \sigma'_{M4} \) at the exit slit. If we denote the length of the entrance arm of the refocusing mirror M4 as \( \delta_{ex-M4} \), and that the exit arm is a sum of mirror to sample \( \delta_{M4-SP} \) and sample to focus \( \Delta \) distances, we get \( \sigma'_{I} = \sigma'_{M4} \cdot \frac{\delta_{ex-M4}}{\delta_{M4-SP}+\Delta} \).

In this case the vertical beam size \( \sigma_v \) at the sample will be the image divergence multiplied by the distance to the focus \( \Delta \), giving \( \sigma_v = \sigma'_{I} \cdot \Delta \). Combining all the previous equations yields that the vertical beam size is given by

\[
\sigma_v = \sigma' \cdot \left[ \frac{\delta_{s-M1} \cdot \delta_{ex-M4} \cdot \Delta}{\delta_{M3-ex} \cdot (\delta_{M4-SP} + \Delta)} \right] \cdot c_{ff}.
\]

Hence, the vertical beam size at the nominal sample position depends on some optical distances (the terms inside the squared brackets), the vertical source divergence and the monochromator magnification.

At the energy range of the beamline the source divergence is defined and dominated by the diffraction limit, which means that it is only energy dependent and cannot be controlled. Moreover, the variation of the source divergence for different photon energies \( h\nu \) does not affect the grating beam acceptance, since the source beam divergence decrease roughly with \( \propto \frac{1}{\sqrt{h\nu}} \) and compensates the increased size due the projection of the beam, which scales with \( \propto \sqrt{h\nu} \) [7].

The results above show that the image size has a linear dependence with \( c_{ff} \) and that it does not depend on the size of the exit slit aperture. This is a consequence of the small dimension of the slit aperture when compared with the optical distances and makes possible to reach the desired photon flux and energy resolution simply adjusting the slit aperture with no effect on the vertical beam size. In addition, through the operation mode (practically the \( c_{ff} \) value) of the monochromator is possible to control the vertical beam size of the spot.
3. Ray-Tracing Simulation
The results of the geometrical description were checked with ray tracing simulations, which were performed with SHADOW through the visual interface ShadowVui at the XOP package [8].

The first step was to determine the distance $\Delta$ between the nominal sample position and the vertical focus. The design criteria was that the vertical dimension must be $150\mu m$ (FWHM) at the chosen reference condition of photon energy $h\nu = 100eV$ and $c_{eff} = 2.25$. The source divergence at 100eV is about $215\mu rad$ (FWHM). Especially here, the use of FWHM is essential as the source has a non-gaussian emission pattern, which in turn is a consequence of the optimization of the undulator $K$ parameter to maximize the photon flux through a large aperture [9, 10]. The vertical beam profile outside the focus actually exhibits a saddle structure (peak to valley difference of $\approx 20\%$ at 100eV) because it is mostly determined by the angular distribution of the photons, but this non gaussian illumination does not compromise the experiments concerned here.

Using the beamline parameters and the geometrical approach presented above, a vertical beam size of $150\mu m$ is obtained with a sample to focus distance of $62.5\, mm$. In simulations the optimal distance turned out to be $62\, mm$, confirming the validity of the approximations used in the geometric description.

As second step, the sensitivity of the vertical beam size regard to the size of the exit slit aperture was checked by the ray-tracing simulation. The slit size was increased ten times from $55\mu m$ to $550\mu m$. As expected, the resolving power decreased by one order of magnitude and the photon flux became higher by one order of magnitude. At the same time, the vertical size increased only by about 15%.

Finally, beam sensitive samples might require a further reduction of the photon density without compromising the total intensity. In this case large apertures are used in the HP-XPS setup and the sample illumination must be changed accordingly. This is achieved by moving the analysis chamber further out along the optical axis. For instance, to create a $500 \times 500\mu m^2$ spot at the sample the setup has to be moved by $150\, mm$ downstream and the monochromator must operate at a $c_{eff}$ value of 5.44 at 100eV.

4. Conclusion
The geometric model shows that the use of astigmatic focusing yields a vertical beam size which is independent of the exit slit aperture and that can be controlled through the monochromator magnification. Ray tracing simulations were performed to verify these results and have confirmed the usability of the astigmatic focusing. Based on these results, we conclude that a single non-bendable toroidal mirror as refocusing element fulfills the requirements set by the HP-XPS experiment. The single mirror solution has been chosen over the conventional KB solution and will be implemented at the forthcoming beamline.

5. References
[1] Follath R, Senf F and Gudat W 1998 J. Synchrotron Rad. 5 769–71
[2] Schnadt J and et al 2012 Journal of Synchrotron Radiation 19 701–704
[3] Aksela S and et al 1994 Rev. Sci. Instrum. 65 831–836
[4] All the sizes and divergences in the text are given as full width at half maximum.
[5] Detailed Design Report on the MAX IV Facility (in preparation)
[6] Palmer C and Loewen E 2005 Diffraction Grating Handbook (Newport Corporation)
[7] Follath R and Schmidt J 2004 (AIP Conf. Proc. vol 705) (Amer. Inst. Phys.) pp 631–634
[8] Meyer B C 2011 (Proc. SPIE vol 8141) ed del Rio M S and Chubar O (SPIE) p 814114
[9] Onuki H and Elleaume P (eds) 2003 Undulators, Wigglers and Their Applications (Taylor & Francis)
[10] Jiang Y H, Püttner R, Martins M, Follath R, Rost J M and Kaindl G 2004 Phys. Rev. A 69(5) 052703