Design of a transmission grating spectrometer and an undulator beamline for soft x-ray emission studies

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\textbf{Abstract.} A soft x-ray undulator beamline and an x-ray emission spectrometer have been designed for soft x-ray emission studies. The beamline has a varied-line-spacing plane grating monochromator, which enables the energy resolution over 10\textsuperscript{4} with a beam size down to 10 \times 60 \mu m\textsuperscript{2}. The x-ray emission spectrometer has a Wolter type I mirror, a free-standing transmission grating, and a back-illuminated CCD. A high collection angle up to 1.5 \times 10\textsuperscript{-3} sr is achieved by utilizing the Wolter mirror as a prefocusing system. The CCD is mounted at 1400 mm downstream of the grating on a Rowland torus mount. Diffracted x-rays are detected in the normal incidence geometry, resulting in high detection efficiency. The energy resolution is limited by the figure errors of the optical elements and the spatial resolution of the detector.

\section*{INTRODUCTION}

High resolution soft x-ray emission spectroscopy (XES) in combination with synchrotron radiation as incident soft x-rays has been extensively studied since the development of a high energy resolution spectrometer by J. Nordgren et. al \cite{1}. The design of their grazing-incidence spectrometer is based on the Rowland circle mount. In this case, the horizontal acceptance angle is mainly limited by the detector size. In order to achieve higher resolution, the Rowland radius, R, or the spectrometer size, should be larger due to the relationship of $\lambda/\Delta\lambda \propto R$. The detector size is however limited. It is therefore desirable to design a novel optical system which can focus the emitted x-rays not only in the (vertical) dispersion direction but also in the other (horizontal) direction. In addition, recent advances make the charge-coupled devices (CCD) a promising soft-x-ray detector. It is however not a trivial problem to adopt it in the high resolution Rowland spectrometer, since the CCD detectors have low quantum efficiency at the small grazing-incidence angle. In this report, we propose a novel spectrometer design for high resolution soft x-ray emission studies. The proposed design consists of a Wolter type I mirror, a free-standing transmission grating, and a back-illuminated CCD. The prefocusing Wolter mirror focuses soft x-rays both horizontally and vertically, resulting in a large collection angle. The CCD detector is mounted on a Rowland torus \cite{2} in a normal incidence geometry, which gives high detection efficiency. We will install the spectrometer in a new soft x-ray undulator beamline BL3U on the UVSOR-II ring.

\section*{BEAMLINE BL3U}

A soft x-ray emission spectrometer generally requires small beam size at the sample position, because a smaller opening of the spectrometer entrance slit is needed to achieve higher energy resolution. Such a beam is usually produced by refocusing optics downstream of the exit slit. In our case, the adoption of such refocusing optics is impossible, due to the very limited space. On the other hand, a monochromator with short arm lengths is utilized with a small exit-slit opening for obtaining practical resolution. It is feasible to carry out XES studies at the exit-slit position, if the monochromator has a constant exit-arm length. We have designed a varied-line-spacing plane (VLSP) grating monochromator in order to satisfy high energy resolution of $\lambda/\Delta\lambda=10^7$ and small width of the exit-slit opening. Figure 1 represents the layout of the beamline BL3U at the UVSOR facility. The in-vacuum plane...
undulator composed of 50 periods of 3.8 cm period length is installed in a straight section, where the electron beam parameters are \( \sigma_x = 602 \, \mu \text{m}, \sigma_x' = 49.9 \, \text{mrad}, \sigma_y = 61.3 \, \mu \text{m}, \) and \( \sigma_y' = 40.6 \, \text{mrad}. \) The brilliance and total flux calculated by using SPECTRA ver. 7.0.5 [3] are shown in Figure 2. The cylindrical mirror M0 vertically focuses the beam on the entrance slit S0 with the demagnification of 1/7.57. The typical beam size at the entrance slit S0 is a full width at half maximum (FWHM) of 22 \( \mu \text{m}. \) Due to the short arm length, the entrance-slit opening corresponding to the resolving power of \( \lambda/\Delta \lambda = 10^4 \) becomes smaller than the beam size. This mismatch causes the beam loss of 12-63%.

Varied-line-spacing parameters are calculated by minimizing the aberrations in the energy range of interest. The analytical solution of the aberrations for an S0-M1-VLSP-S1 optical system derived by Amemiya et. al. [4] is used. The obtained parameters give resolving power higher than \( \lambda/\Delta \lambda = 10^4 \) in the photon energy range of 50-800 eV by using three interchangeable gratings with the center groove densities of 1200, 600, and 240 l/mm.

In the XES setup of Figure 1, the beam is horizontally focused on the exit slit by a plane-elliptical mirror M2X, which is located downstream of the VLSP gratings. A sample is placed at 5-10 mm downstream of the exit slit S1X. In the multi-purpose setup, the beam is focused on the exit slit S1 only vertically and then refocused in the both directions on the sample by a toroidal mirror M2. The M2X mirror and the exit slit S1X are designed to be easily interchangeable with the exit slit S1. The photon flux at the sample position in the multi-purpose setup calculated by using the SHADOW code [5,6] is shown in Figure 2. Here the reflectivity of the gold coating used for all the optical elements, and the grating efficiency are taken into account. The XES setup is also calculated to have very similar flux. In 50-70 eV region, the flux is mainly lost at the grating because the illuminated length is larger than the grating length of 190 mm. In the XES setup, the beam on the sample has a gaussian distribution with FWHM of 60 \( \mu \text{m} \) horizontally. The vertical beam size is close to the opening of the exit slit S1X. Although the beam is diffracted by the exit slit S1X, the vertical size of the beam can be down to \( \sim 10 \, \mu \text{m} \); in the multi-purpose setup, the beam size at the sample position is typically 30(v) \times 170 (h) \mu \text{m}^2.\]

In summary, we have designed the soft x-ray beamline BL3U, equipped with the VLSP grating monochromator having short arm lengths. It is found that the photon flux over \( 10^{11} \) photons/sec is achievable under \( \lambda/\Delta \lambda = 10^4 \) in the photon energy range of 50-600 eV.

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**FIGURE 1.** Schematic layout of the BL3U at UVSOR-II. The distances along the beam from the center of the in-vacuum plane undulator are shown in mm. S1X and M2X can be replaced with the other exit slit S1 so that experiments can be carried out at either the XES or multi-purpose endstation. In XES setup, the sample is placed at 5-10 mm downstream of S1X.

**FIGURE 2.** Brilliance and total flux of the in-vacuum plane undulator (left) and calculated flux at the sample position in multi-purpose setup with the resolving power of \( \lambda/\Delta \lambda = 10^4 \) (right).
DESIGN OF A NOVEL TRANSMISSION-GRATING SPECTROMETER (TGS)

Figure 3 shows the schematic layout of a transmission-grating spectrometer (TGS). In order to focus the emitted x-ray both horizontally and vertically, a Wolter type I mirror is introduced as the prefocussing mirror with a magnification of 10. The Wolter mirror consists of hyperboloidal and elliptical surfaces. The grazing-incidence angle of 1 degree gives a collection angle of $1.5 \times 10^{-3}$ sr. A free-standing transmission plane grating with its groove density of 10 000 lines/mm is placed at 67 mm downstream at the edge of the Wolter mirror, in the normal incidence geometry. A back-illuminated CCD, of which the position is changed along the Rowland torus with scanning the photon energy, is located at 1400 mm downstream from the grating.

![Figure 3. Schematic layout of the transmission-grating spectrometer (TGS) (left). A cross sectional view is also shown (right).](image)

The SHADOW code [6] has difficulties in ray-tracing the present TGS, because it is designed for standard x-ray optical systems. For evaluating the aberrations of TGS, a ray-tracing code TGSGUI is originally developed by one of the authors (T.H.). TGSGUI is a sequential ray-tracing code written in C++. A ray-trace kernel is written to be portable. Owing to the dynamic allocation and a fast and robust random generator [7], TGSGUI is capable of ray-tracing a large number of rays very rapidly. In the present optics, 2.5 million rays are calculated within 27 sec on a personal computer (Pentium III 1.2 GHz). In order to avoid any confusion in the definitions of the optical parameters, most of the definitions for the parameters are identical to those in the SHADOW code. The Igor Pro [8] is used as a graphical engine, for visualizing the obtained results. Users can analyze the results by simply clicking buttons in TGSGUI, which sends commands via DDE communication to the Igor Pro.

In the case of the Rowland circle spectrometers, the horizontal astigmatic aberration is very small because they do not focus the beam horizontally. On the other hand, the Wolter mirror has considerable amount of the astigmatic aberration. Figure 4 presents a spot diagram at the detector position for the 0th order diffraction with a rectangular source of $1(v) \times 200(h)$ µm². This result suggests that the astigmatic aberration is negligible for this source size. Figure 4 (center) shows dependence of vertical standard deviations ($\sigma$) of the rays at the detector on the horizontal source length. The astigmatic aberration increases rapidly with increasing the horizontal length of the source. The present TGS therefore demands small beam size on the sample, both in the vertical and horizontal directions. The horizontal length of the source should be chosen according to the desired energy resolution. In practical operation, this is accomplished by selecting the region of interest on the detector since the horizontal image on the detector is a magnification of the source. Figure 4 (right) indicates a spot diagram of the 1st order diffracted rays of 320 eV at the detector with a rectangular source of $1\times200$ µm². Other aberrations arise from the plane figure of the grating [2]. The diagram however indicates that the present TGS has small amount of the aberrations. The resolving power better than 5000 is possible. The spatial resolution of the detector should be very high, which is estimated to be about 1 µm, in order to achieve such a high resolution.

The Wolter mirror with hyperboloidal and elliptical surfaces was developed and examined by Hamamatsu Photonics K.K. The mirror was manufactured by using the replica method, of which the quality was tested by measuring an image of a zone plate. The image was taken by using an x-ray zooming tube. The groove period of 1 µm is clearly resolved, which corresponds to a point spread function with FWHM smaller than 10 µm. This performance is sufficiently adaptable for the present TGS.

A prototype of the transmission grating was manufactured with a groove density of 6250 lines/mm by NTT Advanced Technology Corporation. The schematic structure of the grating and the theoretical absolute diffraction efficiency is demonstrated in Figure 5. Because the tantalum layer absorbs most of the x-rays, the grating acts as an amplitude grating. The absolute diffraction efficiency of the grating measured at BL4B of UVSOR was 1–2% in 200-250 eV region. The poor diffraction efficiency is due to the imperfect etching depth. On the other hand, the ratio of the stray light intensity to the 1st order diffraction is $10^{-3}$, which is low enough for the present application. The same structures will be etched on a silicon wafer along the illuminated circular area. The development of the transmission grating with better quality is now in progress.
As discussed above, a very high spatial resolution of the CCD detector is required for realizing the present system. Very recently, Tsunemi et. al. have succeeded to achieve the sub-pixel spatial resolution of less than 1 µm in the hard x-ray region for a CCD with 12 µm square pixels, by using the centroid calculation of split pixel events [9]. In order to apply this technique to the soft x-ray region, we are developing a low noise readout system compatible with the ultra high vacuum. The readout noise of 3.6 e⁻ rms at 250 kHz/pixel readout rate was already achieved, even for a prototype CCD system. The CCD (e2V CCD-4240 NIMO) with 13.5 µm square pixels, is cooled down to -100 °C with liquid nitrogen in order to reduce the dark current.

In conclusion, we have designed the new undulator beamline BL3U and the TGS for XES studies. The Wolter type I mirror enables a very high collection angle, but the large astigmatic aberration demands small beam size of incident soft x-rays on the sample. The CCD is used in the normal incidence geometry, which realizes high detection efficiencies. A very high spatial resolution is however indispensable for the normal incidence geometry. The novel TGS is very promising because of its large collection angle and high energy resolution, though some technical difficulties remain to be solved. A total system of TGS is now under development.

FIGURE 4. Spot diagram of the 0th order diffraction at the detector with a rectangular source of 1(v)x200(h) µm² (left). Dependence of vertical standard deviation (σ) of the rays at the detector on the horizontal source size is also shown (center). Spot diagram of the 1st order diffracted rays of 320 eV at the detector with a rectangular source of 1(v)x200(h) µm² (right). It turns out that the energy resolving power better than 5000 is possible.

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REFERENCES

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