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A high-efficiency and high-spectral-resolution EUV/soft X-ray monochromator based on off-plane diffraction

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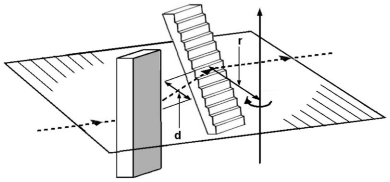
The most efficient diffraction at a periodic grating structure is expected to take place when the incident radiation can be considered to have been specularly reflected off the inclined part of grooves that are positioned parallel to the trajectory of the incident beam. Very encouraging results for this configuration, in which the diffraction takes place off-plane, have been reported recently for a grating to be used in a spectrometer for space science investigations. This grating provided high efficiency for a relatively large groove density and a large blaze angle. High efficiency was observed even in higher diffraction orders up to the fourth order. Here the performance parameters, especially for the combination of diffraction efficiency and achievable spectral resolution, will be discussed for a grating used in a grazing-incidence plane-grating monochromator for monochromatization of synchrotron radiation in the extreme ultraviolet (EUV) and soft X-ray range with photon energies between 30 eV and 2000 eV. It is found that the instrument can provide competitive spectral resolution in comparison with the use of in-plane diffraction. In the case of comparable spectral resolution, the off-plane diffraction is found to provide superior efficiency.

1. Introduction

The highest diffraction efficiency for monochromatization using diffraction gratings is expected when the diffracted wavefronts do not contain any significant discontinuities. In fact, discontinuities may not necessarily lead to a reduced diffracted intensity but they may direct this intensity into more than one diffraction order, which leads to an undesirable diffraction efficiency reduction in a monochromator. It is mostly shadowed regions on the substrate that lead to interruptions in the intensity distribution in the planes of equal phase of the diffracted wave. Such shadows are almost always present when the grating is positioned for in-plane diffraction, *i.e.* when the diffracted beam is found in the plane spanned by the incident and the specularly reflected beam [see, for example, Jark (2019)]. On the other hand, such shadows can be mostly eliminated when the beam trajectory is parallel to the ruling of the grating (Greig & Ferguson, 1950). Optimally the grating profile should then be a staircase, and the exit direction for the diffraction order of interest should simply correspond to the specular reflection at each step, as is depicted in Fig. 1 for a ray being diffracted at the position angle β with respect to the dashed line, which lies in the plane normal to the surface and parallel to the grooves. In fact, in this condition, *i.e.* the so-called blaze maximum, the best directional diffraction is observed, resulting in the highest diffraction efficiency for a single order (Werner & Visser, 1981). In this orientation the diffraction takes place off-plane



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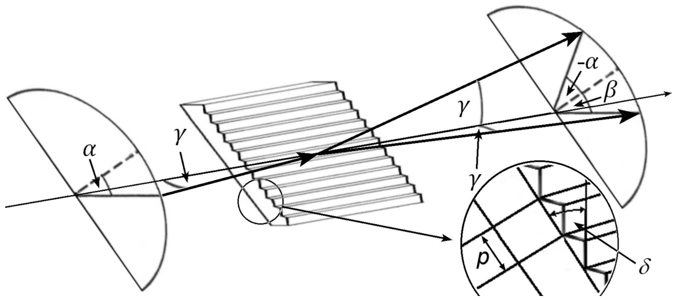

Figure 1
Diffraction of a radiation beam that strikes the inclined surfaces of the grooves of a diffraction grating with periodicity p with an angle of grazing incidence γ. The trajectory of the incident beam is parallel to the grooves and the diffraction takes place off-plane. Then the incident beam at a position angle α and all diffracted orders are found on cones with identical opening angle γ. The specularly reflected beam from the grating surface will be found at position angle $-\alpha$. The grating inclination with respect to the vertical plane is approximately drawn such that the diffracted beam at position angle β progresses in the horizontal direction. The diffraction will take place at blaze maximum when $\beta = \alpha = \delta$, where δ is the grating blaze angle as shown in the inset at the bottom.

and the diffraction orders line up on a cone. In light of the expectedly high efficiency it is now surprising that the off-plane diffraction is used relatively rarely in beamline instrumentation at synchrotron radiation sources; an example is discussed by Frassetto *et al.* (2011). The reason for this could be a common belief that the off-plane diffraction will provide only poor spectral resolution. And thus, when higher spectral resolution is requested, it is common practice to achieve this by use of in-plane diffraction and thus by sacrificing the efficiency of the diffraction gratings in the monochromators. This trade-off can be made when powerful light sources like undulators at storage rings are used. When the sources are weak, however, like stars, a high efficiency is the prime concern in the design of any optics. Consequently most of the development work related to efficient off-plane diffraction is driven by space astronomy (*e.g.* Cash, 1982), and very recently a significant advancement was reported by Miles *et al.* (2018). A staircase grating with an extremely high groove density of $1/p = 6250\ \mathrm{mm}^{-1}$, *i.e.* with a periodicity of $p = 160$ nm, and with a gold coating could provide very high diffraction efficiency in several diffraction orders. For a fixed angle of grazing incidence γ of the light beam of about $\gamma = 1.7^\circ$ with respect to the inclined diffracting surface an absolute diffraction efficiency of 65% was observed for diffraction into the first order at blaze maximum at a photon energy of 380 eV. In the same orientation the fourth order was found to be diffracted with a maximum efficiency of 35% at a photon energy of 1140 eV. This performance corresponds to very high relative diffraction efficiencies of 90% and of 50%, respectively, when compared with the reflection coefficient for the simple gold coating used at the same angle. The comparably unusual property for use in combination with soft X-ray radiation is a large blaze angle of $\delta = 29.5^\circ$ between the inclined steps and the grating substrate, which makes the profile really appear like a staircase. This study will discuss whether, and eventually how, a grating with the reported parameters can be used in a monochromator for synchrotron radiation, and what performance it would provide in terms of instrument transmission and achievable spectral resolution. The expectations for the latter spectral resolution are calculated for the small source sizes expected to be provided by undulators at the new generation diffraction-limited storage rings.

2. Theoretical considerations

In combination with synchrotron radiation and thus with smaller sources in the vertical direction the grating dispersion will always be applied in the latter vertical direction. The optimum orientation for off-plane diffraction from a grating with a blaze angle of $\delta = 29.5^\circ$ is approximately as shown in Fig. 1. In general the grating equation for monochromatization of a wavelength λ by use of off-plane diffraction into the order m reads (Werner & Visser, 1981)

$$\frac{m\lambda}{p} = \sin\gamma\,(\sin\alpha + \sin\beta), \tag{1}$$

where the angles α and β refer to the position angles of the incident and of the diffracted radiation with respect to the plane, which is parallel to the grooves and perpendicular to the grating surface. The earlier-mentioned photon energy E and wavelength λ are related via $E\ [\mathrm{eV}] = 1239.852/(\lambda\ [\mathrm{nm}])$. The incident beam as well as the diffracted orders will be found on cones with the same opening angle γ. Maximum efficiency, or blaze maximum, is observed for $\beta = \alpha$, when $\delta = \alpha$, while the zeroth-order diffraction, *i.e.* the specular reflection at the grating surface, takes place in the direction $-\alpha$. It is now assumed that the source is rather small and that the beam is collimated prior to impinging onto the grating. When the dispersion is then calculated with respect to the position of the specularly reflected peak as derived by Cash (1982), the resolvable bandwidth can be calculated simply as (Jark, 2016)

$$\Delta\lambda = \frac{p}{m}\Delta\alpha, \tag{2}$$

in which case $\Delta\alpha$ is the residual angular spread in the dispersion direction after the beam collimation. The latter spread is caused by the small finite size of the source in this direction, and thus equation (2) refers to the source-size-limited bandwidth.

Actually the monochromated lines will be slightly tilted with respect to the source, as shown by Cash (1982). However, this plays a role only when the source is large in the not-dispersive direction. Here an only slightly elongated source will be assumed, in which case the tilt can be ignored as it will not affect the bandwidth appreciably. In any case the exit slit could always be tilted accordingly for minimizing the related bandwidth deterioration (Cash, 1982).

For comparison, the grating equation in classical in-plane diffraction can be obtained from equation (1) by simply assuming that the opening angle γ of the cone is 90°, and thus it reads

$$\frac{m\lambda}{p} = \sin\alpha + \sin\beta. \tag{3}$$

In this case, blaze maximum for a blaze angle δ is realized for the condition $\beta = -\alpha + 2\delta$. For in-plane diffraction, the blaze angle is usually chosen to be rather small, and thus the grating equation can be approximated as

$$\frac{m\lambda}{p} = \cos\alpha \sin 2\delta. \tag{4}$$

Equation (1) instead reads for blaze maximum $m\lambda/p = \sin\gamma 2\sin\delta$ and thus the latter equation and equation (4) become very similar when $\cos\alpha$ is substituted by the equivalent $\sin\varphi$ for the grazing-incidence case at an angle $\varphi = 90° - \alpha$. The achievable source-size-limited bandwidth is then calculated as

$$\begin{aligned}\Delta\lambda &= \frac{\partial}{\partial\alpha}\lambda\Delta\alpha = \frac{\partial}{\partial\alpha}\frac{p}{m}(\sin\alpha + \sin\beta)\Delta\alpha \\ &= \frac{p}{m}\cos\alpha\Delta\alpha = \frac{p}{m}\sin\varphi\Delta\alpha. \end{aligned} \tag{5}$$

In equation (5), when compared with equation (2), one finds the factor $\sin\varphi$, which is rather small and whose absence in equation (2) is considered to limit the achievable spectral resolution in off-plane diffraction.

3. Discussion

Now the encouraging aspects of the study of Miles *et al.* (2018) are the feasibility to use a rather large inclination angle α in equation (1) as well as a significantly reduced period p in equation (2), and most importantly to use higher orders up to or even beyond $m = 4$. This combination promises to lead to a significantly improved spectral resolution from such a grating when the latter is expressed in terms of spectral resolving power RP = $\lambda/\Delta\lambda = E/\Delta E$.

3.1. Source parameters

The ideally achievable performance will now be discussed in more detail for an undulator source at a diffraction-limited storage ring. The insertion device of length D is assumed to be operated slightly detuned to provide maximum flux in an aperture of finite size. According to Coisson (1988) the σ parameter for the roughly Gaussian-shaped emission angle is then given by

$$\sigma' = 1.3\,(\lambda/D)^{1/2} \tag{6}$$

in both directions. The source size is diffraction-limited in the vertical direction with

$$\sigma_y = 0.15\,(\lambda D)^{1/2}. \tag{7}$$

The full width at half-maximum (FWHM) is 2.35-fold larger in both cases. In the following discussion an undulator length of $D = 4.5$ m and a distance of a beam collimation mirror from it of $L = 22$ m will be assumed.

3.2. Grating parameters

The expected performance data will now be discussed depending on photon energy E and for optical components without any shape errors. For the indicated parameters (p = 160 nm, $\delta = 29.5$, $m = 1, 2, 3, 4$) the on-blaze working curves $\gamma = f(E)$, according to equation (1) for $\beta = \alpha = \delta$, are superimposed in Fig. 2(*a*) onto the plot of iso-reflectivity lines for a gold coating. Such curves can be calculated, for example, by use of the Center for X-ray Optics database (CXRO, 2019). One sees that the parameter set covers optimally the spectral ranges of extreme ultraviolet (EUV) from 30 eV and of soft X-ray radiation from 200 eV up to a photon energy of 2000 eV. In Fig. 2(*b*) the corresponding reflection coefficients R are plotted. From the comparison one expects to find acceptable high diffraction efficiencies at steeper angles of grazing incidence γ in the EUV up to a photon energy of 200 eV and for diffraction into all of the first three diffraction orders. Instead, at larger photon energies $E > 200$ eV, smaller angles of grazing incidence of below about $\gamma = 2°$ will have to be employed. When the scanning is performed on the blaze maximum working curve, a plane mirror will have to be rotated simultaneously with the grating as discussed by Jark (2016). The inclined part of the grooves then needs to always be parallel to the mirror surface, as indicated in Fig. 3. As mentioned in the *Introduction*, the relative diffraction performance of the grating tested by Miles *et al.* (2018) lacks appreciably behind the reflectivity R(Au) of a gold coating. Here the efficiency reduction will be approximated by

$$e = R\,\min\left[0.9,\,\left(300\,[\mathrm{eV}]\,/E\right)^{1/2}\right], \tag{8}$$

where e is the diffraction efficiency and min[a, b] refers to the minimum of the two factors a and b. The latter expression describes well the results presented by Miles *et al.* (2018). The expected transmission T through the optics pair is then

$$T = Re, \tag{9}$$

and is presented in Fig. 2(*c*) for the experimentally investigated first four diffraction orders.

The source-size-limited spectral resolution according to equation (2) was verified with systematic ray-tracing calculations by use of the *SHADOW* software developed by Sanchez del Rio *et al.* (2011). In these calculations also the focus tilt as predicted by Cash (1982) was verified, as was the feasibility to obtain the source-size-limited spectral bandpass by properly tilting the slit. Here also the diffraction limit (DL) for the spectral resolving power, *i.e.* DL = mN (Born & Wolf, 1980), where N is the number of illuminated grooves at the grating, needs to be considered. The related calculations for an undulator source at a diffraction-limited storage ring with the parameters according to equations (6) and (7) are presented by Jark (2019) for in-plane diffraction. Jark finds that the diffraction limit for the spectral bandpass is always only about 10% smaller than the source-size-limited spectral bandpass. It can be shown that the same ratio will be found for off-plane diffraction. Then in both grating orientations the achievable

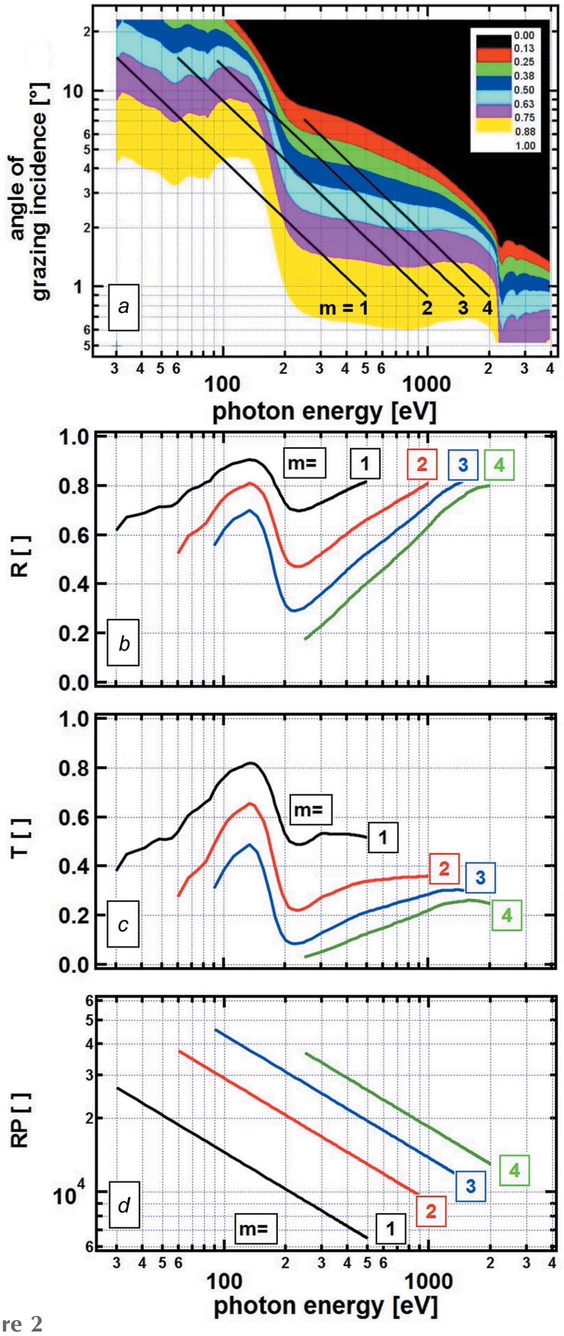

Figure 2
Properties as a function of photon energy of a grating diffracting an incident beam off-plane as shown in Fig. 1 for the first four diffraction orders *m*. In (*a*) the operation angles γ according to equation (1) for blaze maximum operation of a grating with blaze angle δ = 29.5° are superimposed onto color-coded iso-reflectivity curves for a gold-coated grating (see color bar at upper right). In (*b*) the related reflection coefficients for a perfect mirror are shown, while in (*c*) the transmission of a plane mirror/grating pair according to equation (9) is presented, which also includes the observed reduction of the diffraction efficiency according to equation (8). The related spectral resolving powers according to (2) including the diffraction broadening are shown in (*d*).

spectral bandpass will be about 1.4-fold larger than the source-size-limited spectral resolution. The respective line broadening is considered here in the spectral resolving power, RP = $\lambda/\Delta\lambda = E/\Delta E$, reported in Fig. 2(*d*). From Figs. 2(*c*) and 2(*d*) one finds very favorable conditions for the grating operation in the EUV range with spectral resolving powers RP > 35000 for diffraction in the third order with still more than 45% expected efficiency. And even at larger photon energies in the soft X-ray range spectral resolving powers of the order of 15000 can be obtained for higher orders with still a decent efficiency.

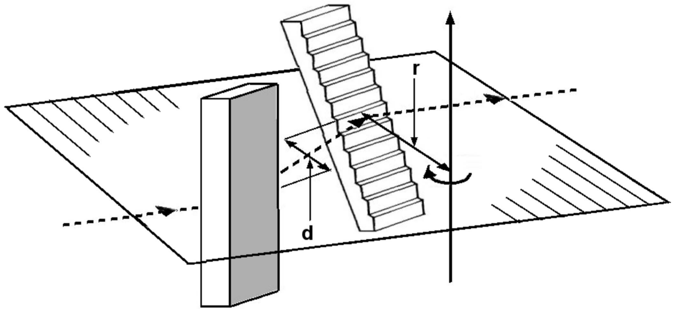

Figure 3
Orientation of a plane mirror/grating pair, in which the inclined grooves are parallel to the surface of the mirror. The plane of incidence for the plane mirror containing the incident and the specularly reflected beam (dashed lines with arrows) is drawn. This plane contains also the diffracted beam from the grating (concluding dashed line with arrow). A vertical rotation axis is proposed to be centered in the incident beam and to be at a distance *r* from the center of the beam footprint at the grating. The mirror surface and the grooved grating area, which intercepts the center of the reflected beam, are separated by *d*. The indicated direction for the rotation will lead to increasing photon energy during tuning.

3.3. Comparison of performance parameters for off-plane diffraction and for in-plane diffraction

In order to put the result into perspective a comparison between the expected performance for in-plane and for off-plane diffraction will be made for the photon energy E = 124 eV (λ = 10 nm), where the transmission is the highest. Fig. 4 presents as points the optimally achievable efficiencies for the first three orders for off-plane diffraction from the test grating according to Fig. 2(*b*), as a function of the optimally achievable diffraction-broadened spectral resolving power RP from Fig. 2(*d*). The line refers to the same correlation for in-plane diffraction, where now the grating periodicity is varied from left to right between about p = 3333 nm and p = 400 nm, respectively. The in-plane diffraction is assumed to take place at the same position and in-blaze operation is assumed at each point. Maystre & Petit (1976) showed, in a comparison with more complex rigorous calculations, that the efficiency for in-blaze operation of a diffraction grating with a staircase profile can be predicted for the first diffraction order with little error simply by use of

$$e_{\max} = R\left(\frac{\phi+\theta}{2}\right)\frac{\phi}{\theta}. \qquad (10)$$

This equation was applied here and its usefulness for the optimization of soft X-ray monochromators is discussed in more detail by Jark (2019). From the comparison in Fig. 4 one finds that for in-plane diffraction eventually better spectral resolving power is feasible than for off-plane diffraction.

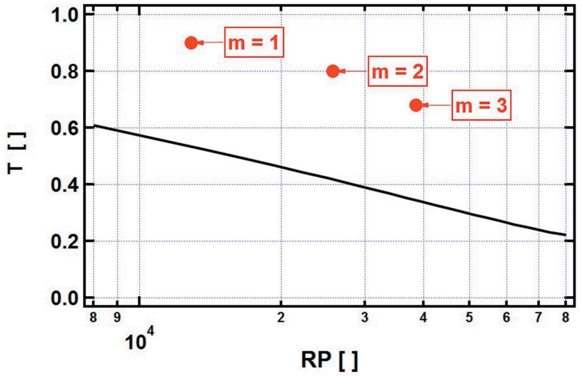

Figure 4
Correspondence between achievable diffraction efficiency and related diffraction-broadened spectral resolving power. The points present the achievable diffraction efficiency for off-plane diffraction according to Fig. 2(*b*) from the tested grating for a photon energy of $E = 124$ eV for the first three diffraction orders m as a function of the achievable spectral resolving power RP according to Fig. 2(*d*). The line presents the same aspect for in-plane diffraction, in which case the groove density can also be varied. Thus for a given spectral resolving power the presented diffraction efficiency is the ultimately possible diffraction efficiency for in-plane diffraction.

However, it can be provided only by use of gratings with large groove densities $1/p$, which provide rather small efficiencies in agreement with practical experience and with expectations (Jark, 2019). Instead, for an identical resolving power, the efficiency for off-plane diffraction expected for smaller photon energies from the test grating always exceeds the efficiency that can be provided for in-plane diffraction.

3.4. Special properties of a related monochromator

A possible scheme for a monochromator utilizing off-plane diffraction is presented in Fig. 5. A plane grating with constant groove density can be used when the incident beam is collimated by a paraboloid (Werner & Visser, 1981). Another focusing paraboloid is needed in order to select the monochromated wavelength in an exit slit of limited opening. Alternative optical schemes are discussed in more detail by Cash (1983) and by Jark (2016). It is evident from Fig. 5 that all optical components in the proposed optical design can be operated with vertical surfaces and with beam deflection in the horizontal direction. In fact the beam trajectory can be kept in a horizontal plane. As the beam is then focused in the direction of the beam dispersion at all components in sagittal focusing, the achievable spectral resolution is much less subject to deterioration due to shape errors than it is in the case of in-plane diffraction, as discussed by Jark (2016). The performance of the presented off-plane diffraction system is also significantly more immune to floor and component vibrations in the vertical direction, which is the principal direction for eventually observed vibrations in synchrotron radiation laboratories, as discussed by McNulty *et al.* (1996).

For improved stability in instrument operation, a reduction of the required scan motions to a minimum is highly desirable. As done for other plane-grating monochromators (*e.g.* Petersen *et al.*, 1995), the use of a long plane mirror simply rotated around a fixed rotation axis is to be preferred over systems in which an additional translation is required. In fact, in the present optical scheme both components need to be scanned simultaneously, keeping the inclined grooves parallel to the surface of the plane mirror. This could be achieved with a single rotation axis, for which a possible positioning is shown in Fig. 3. In this case the rotation axis is vertical and lies in the center of the incident beam. For a horizontal beam displacement by, for example, 20 mm, the center of the beam footprint at the inclined grating needs to be positioned at a distance of about $r = 20$ mm from the rotation axis. In this condition the surface of the plane mirror and the grating need to be separated by $d = 10$ mm. Then the rotation axis will lie 10 mm below the mirror surface and during tuning the beam footprint will move along the mirror surface. It can be shown that as long as small angles $0.9^\circ < \gamma < 2.0^\circ$ are used for operation in the soft X-ray range, after passage through the optics pair of fixed separation, the variation of the horizontal displacement remains smaller than the source size, assumed to be of the order of 0.05 mm in this direction. For operation at smaller photon energies eventually the grating surface may have to be translated by smaller amounts with respect to the common rotation axis. The choice of the indicated position for the rotation axis offers a very convenient way for directing the dispersed beam into a different direction. In fact, after rotating/flipping the entire optics block by 180° around an axis coinciding with the axis of the incident beam, the exiting beam has changed its horizontal position by about 40 mm. At this point it could be incident onto a stationary independent mirror/slit system and it could progress well separated from the alternative trajectory to an independent experimental station. In this scheme there is no requirement to reposition any other optical component.

The simultaneous presence of several operation curves in Fig. 2(*a*) makes obvious a severe drawback in the operation of

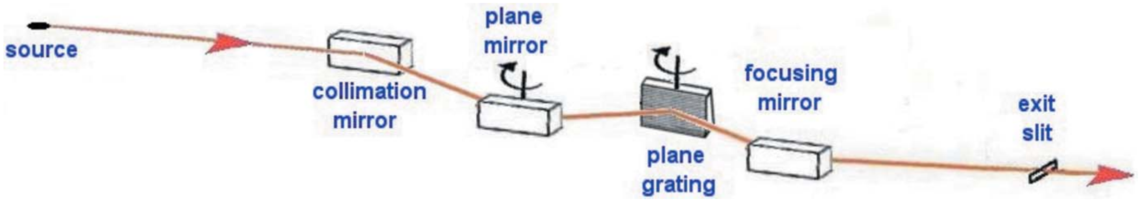

Figure 5
Optical scheme for a grazing-incidence monochromator in which a plane mirror/grating pair will diffract a collimated beam in blaze maximum mode of off-plane diffraction in the horizontal direction. The beam trajectory between the source and the exit slit is from left to right. The indicated combined rotation of the plane mirror and the grating will lead to increasing photon energy.

the described optical system, especially for photon energies beyond 300 eV. At any angle setting $0.9^\circ < \gamma < 2.0^\circ$ a fundamental photon energy will be diffracted with high efficiency, as will be several integer multiples of it. For diffraction up to at least the fourth order the mirror/grating pair does then not have any significant inherent higher-order suppression capability. This will be a severe problem at sources emitting a continuous spectrum. Then other means, such as independent higher-order suppressors based on filter/mirror combinations as described by Sokolov *et al.* (2018), need to be employed in order to reduce such unwanted false light efficiently. The situation is more favorable for undulators at synchrotron radiation sources, which emit a line spectrum. Also this spectrum contains higher harmonics, which are integer multiples of a fundamental photon energy. Much of the unwanted false light contributions can then be filtered by a proper choice for the combination of undulator harmonic and grating diffraction order. Such optimization will have to be made case by case as it depends on the chosen spectral range for the monochromator and on the parameters for the undulator as well as on the electron beam energy.

4. Conclusion

It has been shown that the parameters for a recently tested grating (Miles *et al.*, 2018) for efficient off-plane diffraction can provide, in an appropriately designed optical instrument for synchrotron radiation sources, rather competitive spectral resolving powers with superior transmission in comparison with the use of less efficient in-plane diffraction. As any beam deflection in the optical instrument takes place in the horizontal direction, and thus orthogonal to the direction of wavelength dispersion, the system can tolerate larger shape imperfections than can an instrument that uses in-plane diffraction. Likewise, the system performance will be less affected by vibrations in the vertical direction. A special problem will be higher-order suppression, as such orders are efficiently diffracted at the grating.

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