Variable line-space gratings: new designs for use in grazing incidence spectrometers

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Variable line-space gratings: new designs for use in grazing incidence spectrometers

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Spectroscopy is one of the fundamental techniques in astronomy. However, spectroscopic study of sources emitting in the extreme UV (\(\lambda \sim 100-1000\) Å) and the soft x ray (\(\lambda \sim 10-100\) Å) is still in its infancy, in part due to a lack of spectrometer designs suited specifically for grazing incidence optics. We introduce two such designs and variations, which have emerged from a study\(^1\) of spectrometer options for the Extreme Ultraviolet Explorer (EUVE) satellite.\(^2\)

Both designs achieve spectral imaging through a smooth variation in the line spacing across a reflection grating. Although variable line-space gratings at grazing incidence have recently been proposed for monochromators\(^3\) and also demonstrated for laboratory spectrometers,\(^4\) our approach is fundamentally different: (1) the gratings are flat, and (2) they are placed to intercept the converging beam from a collecting mirror rather than the diverging beam from a slit. This results in (a) small aberrations over a wide instantaneous range in wavelength, (b) a modest required variation in line spacing across the ruled width, (c) a simultaneous minimization of both the spectral and image height aberrations, and (d) a completely stigmatic zero order image. The slitless arrangement common to our designs is very compact, having no additional length behind the focal plane of the collecting mirror.

A schematic layout of the first design is shown in Fig. 1(a). The grating is mounted in-plane, and a cross section of the converging beam is shown in the dispersion plane. The simplest solution for the line-space variation, and the one adopted for use on EUVE, is shown in Fig. 1(b). It consists of straight grooves whose spacing \(d(x)\) is varied by a mechanical ruling machine\(^5\) according to the equation

\[
d(x) = m \lambda_0/[\cos\beta(x) - \cos\alpha(x)],
\]

where \(m\) is the spectral order, \(\lambda_0\) is the correction wavelength, and \(\alpha(x)\) and \(\beta(x)\) are the local grade angles of incidence and diffraction. In the limit of small angles \(\alpha\) and \(\beta\), an approximate estimate to the required variation in line spacing is given by \(d(x_{\text{min}})/d(x_{\text{max}}) \approx (\alpha_{\text{max}}/\alpha_{\text{min}})^2\). This variation is modest due to use of a converging incident beam. Equation (1) is simply the local grating equation. The same result for \(d(x)\) has also been obtained through direct use of the light-path function.

\[\text{Fig. 1. Geometry of variable line-space plane grating spectrometer. Collecting mirror is upstream of the converging beam: (a) projection upon the dispersion plane; (b) grating plane having variably spaced straight grooves; (c) variably spaced curved grooves, provided by holographic fabrication.} \]
All rays \( \lambda_0 \) illuminating the grating along line \( AB \) [Fig. 1(b)] are thereby brought to a point focus, whose distance from grating midpoint \( O \) is set equal to the distance \( L_0 \) from that midpoint to the mirror focus. All rays \( \lambda_0 \) illuminating groove \( CD \) thereby have the same path length difference and, therefore, are also brought to this point focus.

Focal plane aberrations at \( \lambda_0 \) will result from other regions of the grating aperture. The error in the light-path function is

\[
\Delta = (m \lambda_0 d_0) \left[ \frac{\gamma x^2 y^2 + \frac{1}{2} x^2 y^2 \cos \beta_0 + \cos \alpha_0}{\cos^2 \alpha_0} \right],
\]

(2)

where \( x \) and \( y \) refer to the coordinate system of Fig. 1 with origin at point \( O \) and all distances in units of \( L_0 \). Note that there is neither astigmatism nor first-type (tangential) coma, the lowest-order terms being second-type (sagittal) coma and spherical aberration. Converting this wavefront error to image aberrations at the focal plane, we find the resolving power \( \lambda/\Delta \lambda \approx 8 f_0^2 \) and the image height \( H \approx (L_0/2)(m \lambda_0/\lambda_0)(\alpha_{\max} - \alpha_{\min})/\alpha_{\max}/f_y \), where \( f_y \) is the effective focal ratio of the illuminating beam in the \( y \) direction.

If this resolution is to be attained, the grating dispersion must overcome any angular uncertainty \( (F/F_0) \) incident to the grating, where \( \epsilon \) is the image quality (in seconds of arc) of the collecting mirror, which has focal length \( F \). At the focal plane, this uncertainty is converted into a wavelength blur:

\[
[\Delta \lambda]_{\text{dispersive}} = 5 \times 10^{-6} (d\lambda/ds) F \epsilon (\sin \alpha/\sin \beta),
\]

(3)

where \( (d\lambda/ds) \) is the plate scale. Use of negative (or inside) spectral orders, for which \( \sin \alpha < \sin \beta \), thus minimizes the wavelength aberrations due to finite \( \epsilon \), for a given plate scale. The ratio \( \sin \alpha/\sin \beta \), or its reciprocal, is also equal to the peak diffraction efficiency of a blazed grating. We find the inside spectral orders to provide for higher diffraction efficiency (and a broad range) at a given spectral resolution, becoming an increasingly significant effect at higher dispersion. At normal incidence, for which \( \sin \alpha \approx \sin \beta \approx 1 \), such differences between \( m > 0 \) and \( m < 0 \) are usually not apparent. Adjusting the dispersion to maintain \( \lambda/\Delta \lambda = 8 f_0^2 \) across the spectrum, we find \( H \approx 2 \times 10^{-9} F f_y (\alpha_{\max} - \alpha_{\min}) \lambda_0/\lambda_{\min} \).

Figure 2 shows a ray trace of the grating with an \( f/5 \), \( \epsilon = 1 \) grazing mirror, and a flat detector. For this example, the grating was placed to intercept \( 1/6 \) of the beam at a distance \( L_0 = f/5 \) from focus. Thus \( (\alpha_{\max} - \alpha_{\min}) \approx \lambda_0/\lambda_0 \) and \( f_y \approx 10 \), leading to predicted grating aberrations of \( H \approx 4 \times 10^{-5} \) and \( \lambda/\Delta \lambda \approx 800 \). The actual ray trace, including mirror blur, shows \( H \approx 2 \times 10^{-5} \) and \( \lambda/\Delta \lambda \approx 700-1100 \). These results are slightly better than predicted, due to the grating aperture being underilluminated by the (annular) mirror beam.

Apparent in Fig. 2 is that the instantaneous spectral coverage is potentially very large (100–1000 Å). This results because the \( \lambda = 0 \) (\( \epsilon = 0 \)) image is stigmatic, resulting in nearly equal plate scales at \( \lambda_0 \) from all points on the grating aperture. Thus aberrations cannot grow rapidly away from \( \lambda_0 \), leading to wide spectral coverage. For ease of calculation, a cylindrical detector of radius \( L_0 \) was centered at point \( O \) on the grating, so as to pass through both the stigmatic point \( m = 0 \) and the correction wavelength \( \lambda_0 \). This choice minimizes all image heights and leads to the spectral range

\[
\lambda_{\max}/\lambda_{\min} = 1 + c \times 10^5 (\lambda/\Delta \lambda)^{-2}(F \epsilon/L_0)^{-1}(\alpha_{\max} - \alpha_{\min})^{-1},
\]

(4)

where \( \lambda/\Delta \lambda \) is maintained across the entire range \( \lambda_{\max} \) to \( \lambda_{\min} \). For the chosen focal surface, \( c = 4 \). This equation underes-
timates that achievable with even a flat detector optimally oriented to minimize wavelength aberrations rather than image heights. For example, it predicts $\lambda_{\text{max}} / \lambda_{\text{min}} \approx 4$ for the system ray traced in Fig. 2, which shows $\lambda_{\text{max}} / \lambda_{\text{min}} = 10$. Of course, in a practical spectrometer the wavelength range is also limited by filter bandpasses and by the curve of diffraction efficiency.

The use of a plane grating results in a stigmatic image at $m = 0$. This is the key to use of photore sist (holographic) methods to improve the above design by generating a completely stigmatic image at $\lambda_0$. Two coherent light sources of wavelength $\lambda_0$ will produce standing waves, for which the light paths differ by an integral number of wavelengths. The interference patterns are hyperboloids of revolution about the axis joining the two source points. Consider these sources to be placed at the focal positions of $\lambda = \lambda_0$ and $m = 0$ and employ a flat substrate coated with photore sist. The resulting interference fringes become curved grating grooves [Fig. 1(c)], which, when illuminated by a beam having the assumed focus, produce aberration-free (stigmatic) images at $\lambda = \lambda_0$ and $m = 0$. The fabrication method can use coherent light of wavelength $\lambda_0$ or possibly de Broglie waves from low-energy electrons of wavelength $\lambda_0$, or conventional UV lasers on an enlarged photore sist subsequently reduced to form the grating mask. The latter scaling process is made possible by the flat grating surface.

For the special case in which the line joining the two sources is perpendicular to the grating plane, the grooves in this plane are concentric circles centered at the point of intersection, and the focal surface is the line joining those sources [extension of the dot--dash line in Fig. 1(a)]. This groove geometry has the unique property that all rays hitting any one groove come to the same point focus, as the path length difference is constant, and this holds for all wavelengths. All image heights thereby vanish, and wavelength aberrations away from $\lambda_0$ are given by Eq. (4) with $c = 2$. Even for the source geometry of Fig. 1(a), circular grooves with varying curvature are found to remove both the comatic and spherical terms in Eq. (2), leaving a residual aberration $\lambda \Delta \lambda \approx (128/3)^4/\lambda_0^4$. The system parameters used above, the grating aberration limit to $\lambda \Delta \lambda$ rises from 800 to $4 \times 10^4$ and is 27,000 if $1/2$ rather than $1/6$ of the beam is accepted by the grating. Particularly for the special case which leads to concentric grooves and complete stigmatic at $\lambda_0$, the required curved grooves represent a simple motion for a mechanical ruling machine. The resulting blazed grating can function as an echelle. Alternately, straight grooves could provide the above correction at $\lambda_0$ if ruled on a nonspherical surface whose curvature is small but follows the patterns indicated for curved grooves.

The fact that holographic recording upon a flat grating surface generates completely stigmatic points at $\lambda = \lambda_0$ and $m = 0$ can be generalized to off-plane gratings and leads us to our second general design. Consider two light sources positioned symmetrically on opposite sides of the in-plane dispersion plane shown in Fig. 1(a). The result is a series of hyperbolic grooves which can be approximated as shown in Fig. 3(b), by straight grooves which radiate from a ruling focus located behind the focal plane. This “oriental fan” geometry is used in conical diffraction and can conceivably be ruled mechanically by a simple motion which rotates the grating sample by equal angles between grooves.

For this extreme off-plane (conical) mount, linear dispersion per unit wavelength is $L/d$, where $L = ds$ is the position of the focal plane and $d = \text{gr} \; \text{ groove spacing}$. The optimal displacement $(\Delta RF)_{\text{opt}}$ of the ruling focus behind the focal plane minimizes the variation of this $L/d$ ratio across the grating aperture:

$$
(\Delta RF)_{\text{opt}} \approx L_0 \sin^2 \gamma_0 \cos \gamma_0
$$

where $L_0$ and $\gamma_0$ are the values of $L$ and the graze angle at the grating center. The fan grating geometry is thus not specific to a particular mounting, so a single grating can be used over a range of incident graze angles, given the constraint of Eq. (5). With this constraint, straight grooves near the center of the grating are tangent to the hyperbolas from a stigmatic holographic ruling. This choice is confirmed by ray tracing, as shown in Fig. 3(b), where $\lambda_0 = 125 \lambda, f_s = 6.3, \gamma_{\text{max}} - \gamma_{\text{min}} = \gamma_0$, and $(\Delta RF)_{\text{opt}} = 19 \text{ mm}$. The wavelength spots are elongated, and $\pm 25\%$ shifts in $\Delta RF$ about the optimal value serve only to rotate the direction of this elongation slightly out of the dispersion direction.

In general, given the ruling focus displacement of Eq. (5), the aberrant light-path function at $\lambda_0$ is

$$
\Delta = (m \lambda_0 / d)(\lambda_{\text{max}} - \lambda_{\text{min}}) / \lambda_0^2 + \cdots / \cos^2 \gamma_0
$$

where all distances are in units of $L_0$. The origin is at the geometric center of the grating, and the $x$ axis lies along the central groove ($\gamma = 0$). Since this groove is everywhere equidistant from the focal plane positions of $m = 0$ and $\lambda = \lambda_0$, all rays $\lambda_0$ hitting this central groove come to a point focus. Therefore, Eq. (6) has no astigmatic term. Converting the wavefront error $\Delta$ to image aberrations at $\lambda_0$, we find an image height $H / L_0 \approx (\lambda_{\text{max}} - \lambda_{\text{min}})^2 / f_s$ and a spectral resolution $\lambda / \Delta \lambda \approx 8 f_s / (1 + f_s^2 (\gamma_{\text{max}} - \gamma_{\text{min}})^2)$. It is apparent in Fig. 3(b) that aberrations in $\lambda / \Delta \lambda$ grow rapidly longward of $\lambda_0$. These can be minimized by a tilt $\phi$ of the focal plane, as defined in Fig. 3(a), resulting in the bottom raytrace of Fig. 3(b).

Each of the above two grating designs (in-plane and conical fan), and variations having curved groves, can be used alone. However, Eq. (4) indicates the spectral coverage to narrow rapidly with increases in resolving power. Using the mirror parameters given above, a $\lambda / \Delta \lambda = 10^4$ leads to a spectral coverage of $\lambda_{\text{max}} - \lambda_{\text{min}} / \lambda_0$ of only $\sim 1\%$ for the in-plane grating design. Fortunately, two variable line-space gratings can be mounted in series, allowing the second grating to separate overlapping echelle orders produced by the first grating. Such an echelle spectrometer covers a wide spectral range at high resolution.

The construction of an echelle spectrometer from these gratings is made possible because the first grating produces a continuum of foci (the dispersed wavelengths), each of which the second grating treats as an (off-axis) mirror focus. Figure 4 shows one possible combination, where highly dispersed wavelengths off an in-plane echelle enter a conical cross-dis perser. (Alternatively, the conical cross-disperser may precede the in-plane echelle, thereby minimizing the spread of graze angles into the second grating.) The cross-disperser aberrations are minimized at the wavelengths off the echelle for which the focal plane is displaced from the (fixed) ruling focus by $(\Delta RF)_{\text{opt}}$, as given by Eq. (5). Given a focal surface which minimizes echelle aberrations and given reasonable values of dispersion, the displacement error $\Delta RF - (\Delta RF)_{\text{opt}}$ at the extreme edges of the spectrum is found to be within the accuracy in determination of $(\Delta RF)_{\text{opt}}$. The latter results from the range in $L \sin^2 \gamma \cos \gamma$ across the grating and was approximately $\pm 25\%$ for the system ray traced in Fig. 3(b). Thus the focal surface for the cross-disperser coincides with that of an echelle, resulting in a $2D$ echellog ram focused upon the detector. This allows a large range in wavelength to be covered instantaneously at the high spectral resolution delivered by the echelle.
As an echelle, the in-plane grating requires a variable blaze angle to maintain blazing in the high orders. The fan grating has a nearly uniform blaze, varying by only a fraction \((\gamma_{\text{max}} - \gamma_{\text{min}})/\gamma_0/2\) across its aperture, but as an echelle requires curved grooves. Thus a second possible combination is to follow a cross-disperser in-plane grating by a conical echelle having curved grooves. Other variations include the use of one grating design (in-plane or conical) for both the echelle and the cross-disperser.

Finally, we note that any of the above designs, including single gratings, can be transformed into a slit spectrometer by use of a relay optic. This optic can also slow the beam convergence, reducing the grating aberrations.

To summarize: we have introduced two new classes of grazing incidence gratings and several variations, which can be used individually or in combination; and have illustrated one combination in the form of an echelle spectrometer. These designs represent ideal candidates for moderate to high resolution spectrometers on such missions as the Far Ultraviolet Spectroscopic Explorer (FUSE, now Columbus) and the Advanced X-Ray Astrophysics Facility (AXAF).

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