THE SINGLE-BEAM WAY TO CONCAVE GRATINGS

BY JAY ZAKRZEWSKI

The optical components in a spectrometer perform two functions. They form an image of the slit through which the light enters the instrument, and they disperse the light into a spectrum so that images of different wavelengths are formed at different positions in the focal plane. In most instruments the image formation is achieved by lenses or mirrors that act as collimator and

An interference technique using a single laser beam, developed at the National Physical Laboratory in England, creates a major advance in concave diffraction gratings.

camera, and the dispersion is achieved separately by either a prism or a grating. Yet it has been known since 1882 that it is possible to combine the two functions in a single component by ruling a diffraction grating directly onto the surface of a concave mirror.

There are two distinctly different advantages to be gained from the use of concave gratings:

1. The instrument consists of far fewer components than one with separate collimator, disperser and focusing elements. It should therefore in principle be less expensive to manufacture and assemble.

2. By avoiding the use of several optical components we avoid the optical losses associated with these components. For visible and infrared radiation these losses are not great, but in the ultraviolet, where the reflectance of metal mirrors may be as low as 10 percent, the use of a concave grating could increase the throughput of an instrument by a large factor.

When contemplating the use of a concave grating it is important to appreciate for what reason you are doing so, because the design philosophies behind ruled vs. interference are quite different. If your objective is to minimize the cost of manufacture, then you require a simple *mechanical* construction. This can be achieved, but usually at the cost of some degradation of optical performance. If you are looking for diffraction-limited optical performance, then you must take great care in setting up the instrument anyway, and a given specification usually can be achieved most easily using separate focusing optics. This does not, of course, apply to the ultraviolet. But here one has to accept a more com-

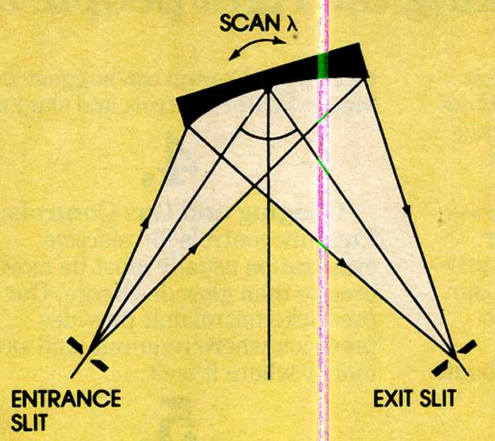

Figure 1.
The Seya-Namioka mounting.

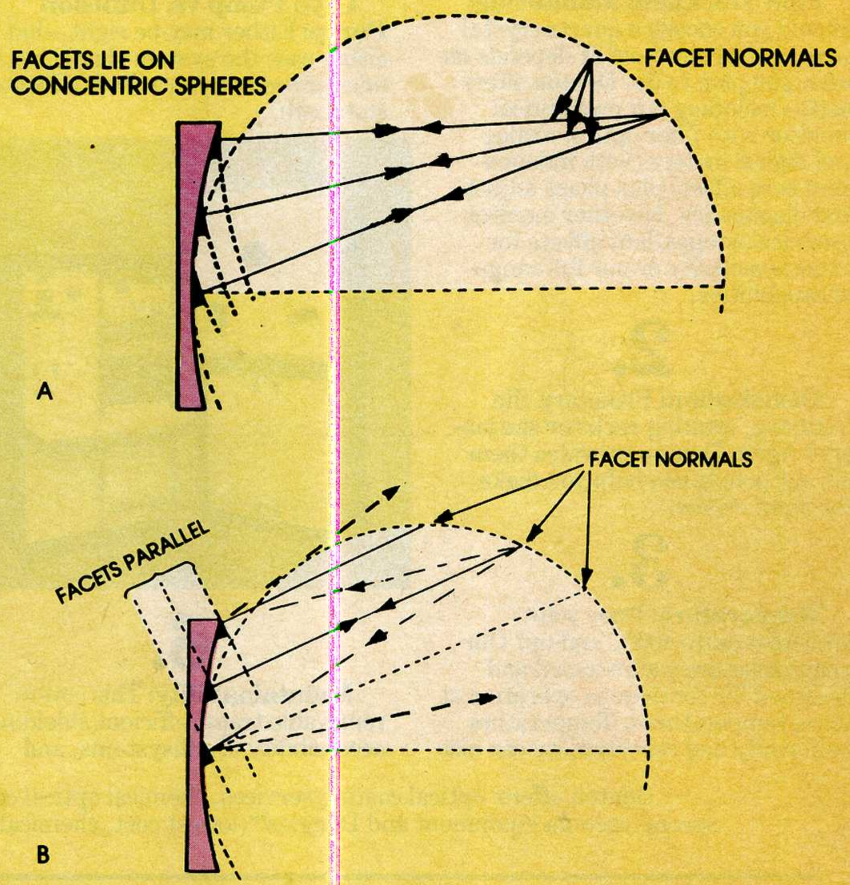

Figure 2.
The ruled concave grating: (a) would form a perfect image, but (b), with parallel facets, manifests reduced efficiency.

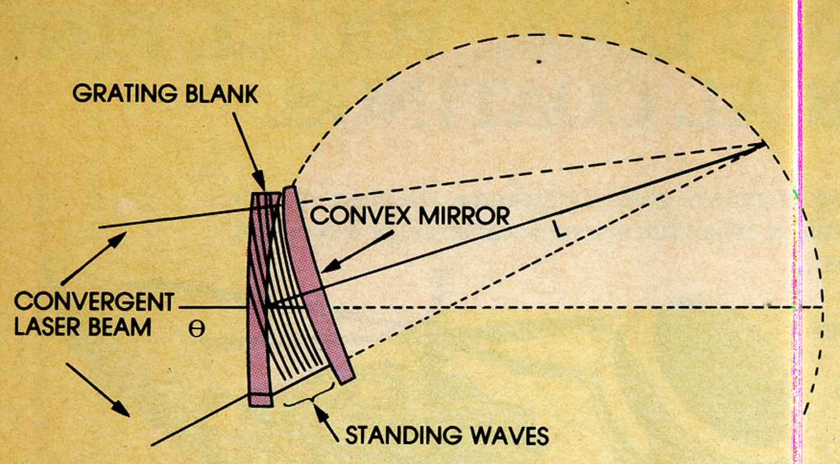

Figure 3.
Recording a concave grating with a single beam.

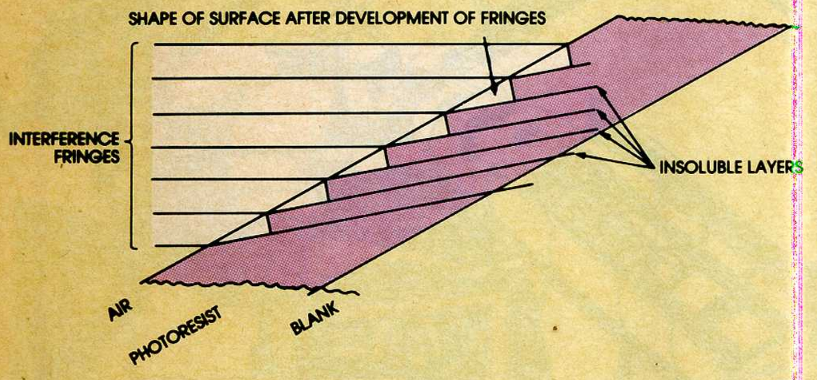

Figure 4.
The blazed groove profile of a concave grating.

plex mechanical arrangement, and under these circumstances the cost is of less importance than the performance of the instrument.

Classical ruled concave gratings

The original form of the concave grating was first made in 1882 by Rowland. He simply substituted a concave blank for a plane one on his ruling engine, so that the spacing of the grooves was constant when projected onto a chord. He also demonstrated that if a source is located on a circle that touches the pole of the grating but has half the radius of curvature of the blank, then the diffracted image lies on that circle (the "Rowland circle").

The fact that the spectrum is formed on a curved surface is a significant practical disadvantage. In a spectrograph it means the photographic plate, or other detector, must be deformed to fit the circle if all wavelengths are to be in focus. Similarly, in a monochromator you must move the grating back and forth as it is rotated because the focal distance varies with wavelength.

A variety of mechanical linkages has been designed by which this motion may be achieved automatically. But these have to be made with some precision, and it is unlikely that such an instrument would be any cheaper to make than one with separate focusing optics. Whether this conclusion remains valid in an instrument that is to be controlled by a microprocessor is open to question. Generally, however, one would prefer simply to rotate the grating.

This condition is achieved in the Seya-Namioka mounting (Figure 1). An instrument based on this design requires only a fixed entrance and exit slit and a simple rotation of the grating. Its one great drawback is that it suffers astigmatism, so that a point source is imaged into a long line. Depending upon the shape of the entrance and exit slits, this leads to a loss of intensity, of transmitted flux and, through slit curvature, of resolution.

A further disadvantage of the classical ruled concave grating is that the facets of all the grooves are parallel. In order to form an image, rays striking different parts of the grating surface need to be sent in different directions as shown in Figure 2a. Thus, if all facets are parallel, only those in one part of the grating can be properly oriented to give the desired blaze characteristics, and the efficiency of the rest of the grating is substantially reduced (Figure 2b).

The development of techniques for producing gratings by recording interference fringes in photoresist added new degrees of freedom to the subject of concave gratings. By choosing the appropriate shape of the wavefronts used to generate the fringes it is possible to make gratings with curved grooves and spacing that varies across the aperture. In this way completely new focal properties may be achieved, and under some circumstances it is possible to produce a perfect image.

The latter can be explained with reference to common holographic terms. The two wavefronts are derived from point sources, one of which is situated at the center of curvature of the blank and may be considered as the "object beam." When the hologram is illuminated with the reference beam it reconstructs the object beam. But, since the grating is coated with a reflecting layer, the substrate reflects the spherical object beam to form a perfect image at the center of curvature.

The holographic argument is valid only if the conditions of "replay" exactly match the conditions of recording. Other geometries and other wavelengths will introduce aberrations, and the image will not be perfect. The very purpose of a grating is that it should be used for more than one wavelength, and if it is to be used at wavelengths that are substantially different from the recording wavelength, then significant aberrations may be expected. These may well be more complex than the aberrations usually encountered with simple optical systems.

This type of grating is made by recording the interference fringes generated at the intersection of wavefronts from two point sources that in principle may be positioned anywhere in space. But the spacing of the fringes at any point is determined by the angle subtended by the two points, and is given by

$$f = \frac{\lambda o}{2\sin\theta}$$

where θ is the *semi* angle between the rays. The pitch of the grating, determined by the spacing of the fringes and by the inclination ϕ of the normal blank to the bisector of the beams, is given by

$$d = \frac{f}{\cos\phi} = \frac{\lambda o}{2\sin\theta\cos\phi}.$$

If the two point sources are at infinity so that the wavefronts are plane and if they are symmetrically disposed to

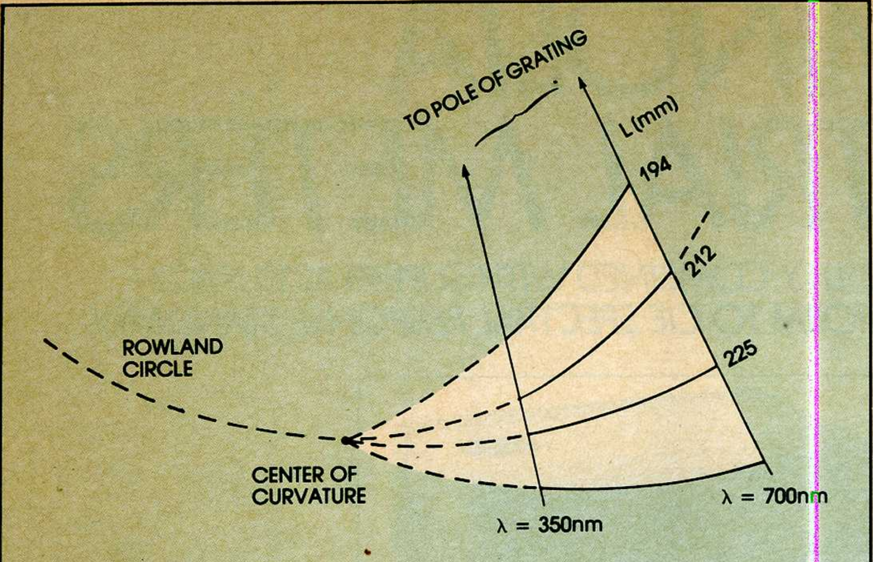

Figure 5.
Focal curves for a series of gratings with 1200gr/mm on blanks of various radii.

the normal of the blank, then the pitch is constant across a chord and is equal to

$$\frac{\lambda o}{2\sin\theta}$$

and the focal properties of the grating are identical to those of a classical ruled grating.

Two-beam concave gratings

If you are prepared to put no restraint on the positions of the recording sources, then you have the flexibility to design a grating optimized for almost any aspect of its performance. A wealth of work has been published in the scientific literature describing gratings designed for a variety of purposes, and it is rather difficult to assimilate it all. The basic design procedure has been summarized in *Diffraction Gratings*,[1] and is summarized more briefly below.

First you set down an expression for the light-path function, which is related to optical path length from source to image via an arbitrary point on the grating surface. This expression is then differentiated with respect to the coordinates of the surface and set equal to zero. This is simply Fermat's condition that for a focus, the light-path functions are the same for rays going via all parts of the grating aperture, thus containing an infinite series of terms that describe the various aberrations of the image.

Each term is a function of the coordinates of the object and image position and of the positions of the recording sources. By setting any chosen term equal to zero, we derive equations from which we can determine the coordinates of the recording sources required to eliminate the corresponding aberration. If these equations are insoluble (i.e., it is not possible to eliminate that aberration completely), we set the differential of that term equal to zero and calculate the positions of the recording sources that give a minimum value for that aberration.

This, however, is only half the story. The procedure we have described enables us to calculate the positions of the point sources used to generate a grating that is optimized according to some chosen criterion. It does not tell us how well that grating will actually behave either in the design configuration or as one departs from it. In order to derive this information it is necessary to perform a ray-trace analysis.

The design analysis determines the position of the sources, from which it is possible to calculate the shape of the grooves of the grating. From this it is possible to calculate the path of any ray from a spectral source diffracted by the grating. This calculation is performed for a bundle of rays, and the points where the bundle intersects the image plane determine the shape of the diffracted image. This calculation must then be repeated for a variety of positions of the source in order to simulate an entrance aperture of finite size (e.g., the entrance slit) and for various wavelengths covering the range over which the instrument is to be used.

Only by performing a ray-trace analysis in this way is it possible to predict the focal properties of the grating. Without such an analysis, there is a risk that in reducing one aberration one may unwittingly incur an unacceptable increase in another.

There is undoubtedly a great deal to be gained from the use of the interference technique in which the positions of the recording sources are carefully chosen to optimize some feature of the focal properties of the grating. Compared with a conventional ruled grating, they may have the following advantages:

1. A low level of stray light;
2. Possibility of higher numerical aperture, since fringes may be recorded on more steeply curved substrates than can be ruled upon;
3. Reduced astigmatism, leading to greater throughput or image intensity;
4. Improved focal curves, leading to simpler construction of instruments.

However, against this one must set the following disadvantages:

1. In a normal two-beam concave interference grating the groove profile is sinusoidal and therefore the efficiency is usually lower than that of a blazed grating. This is because the conditions in which a symmetrical profile leads to high efficiency are often precluded by the constraints of the interference design process.
2. Design requirements often conflict, and it is not usually possible to achieve all the advantages on the same grating. For example, in a modified Seya-Namioka mounting, it may be possible to reduce the astigmatism holographically, but this may introduce coma, which broadens the image and reduces the resolution. Only by performing a full ray-trace analysis is it possible to assess the performance adequately.

Single-beam concave gratings

The single-beam process for producing concave interference gratings is as follows: Rather than record two-beam interference fringes generated by wavelengths from two point sources, this unique process exposes the photosensitive material to standing waves from a single beam. The process is shown diagrammatically in Figures 3 and 4.

Convergent light from a laser passes through the substrate and is reflected back along its own path by a convex spherical mirror. This generates a series of spherical standing waves parallel to the surface of the mirror; these intersect the photoresist surface at an oblique angle. Inside the bulk of the resist the nodal surfaces define regions that are unexposed and therefore insoluble. When the resist is developed the exposed material is removed, but the development tends to stop when it reaches a nodal surface. This results in a grating with a sawtooth or a blazed groove profile.

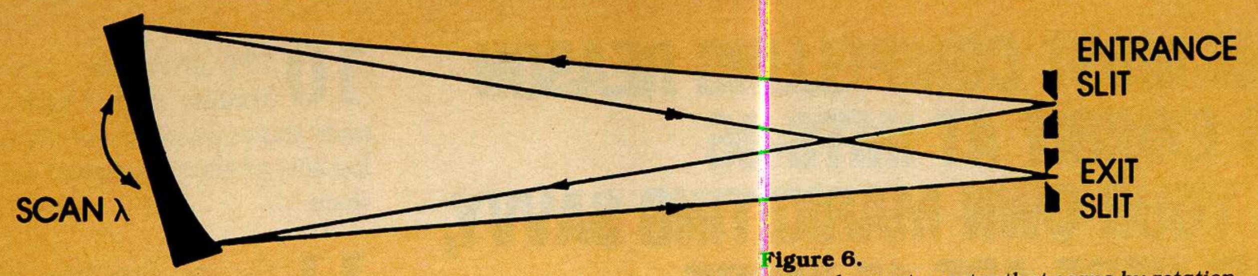

Figure 6.
A simple spectrometer that scans by rotation of the concave grating.

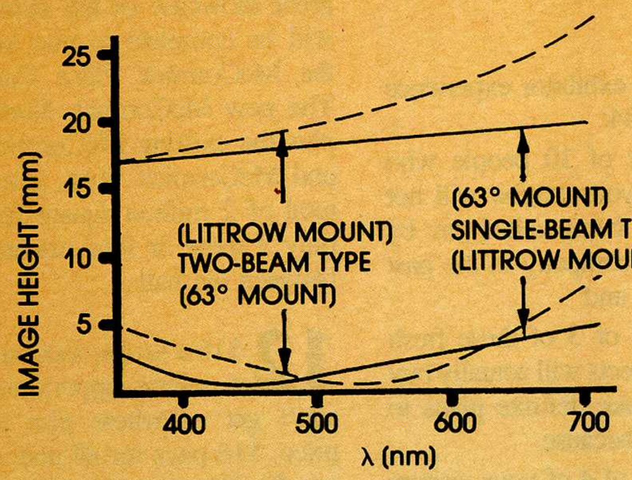

Figure 7.
A plot of the astigmatism from 350-700nm for a 1200gr/mm on a 220nm blank with an aperture of 35mm diameter.

The focal properties of this grating are such that light from a source placed at the point to which the laser light was converging will be diffracted back along its own path and will form a perfect image at the wavelength used to record the grating. Furthermore, all the facets of the grooves are perpendicular to rays diverging from a single point, and the blaze is therefore constant over the whole of the grating aperture.

This type of concave grating therefore offers the following advantages:

- A genuine blazed groove profile that is constant over the aperture, leading to higher efficiencies than with ruled or sinusoidal gratings.
- Very good aberration correction in an Eagle or Littrow type of mounting where the spectral image is formed close to the source, permitting instruments of a compact design.
- High efficiency and low aberrations combined on a single grating without limiting the choice of pitch.
- As with the two-beam concave interference gratings, the capability of a Rowland-circle focal curve and the ability to be made as direct replacements for ruled concave gratings in existing instruments.

There are two limitations:

1. The blaze wavelength produced by the single-beam process is determined by the separation of the standing waves in the photoresist, and this in turn is determined by the laser light's wavelength and the refractive index of the resist. In practice it is possible to generate profiles with a Littrow blaze wavelength of 250nm or less. In the ultraviolet the efficiencies of such gratings are as high or higher than those of the best ruled gratings. At longer wavelengths the efficiencies are lower but still useful. Plane gratings with exactly the same profile are widely used in spectrometers in the visible and near-infrared.
2. Significant reduction of aberrations is only possible in near-Littrow conditions. In other mountings the aberrations are no worse than those of a conventional ruled grating, but where there is a large angle between the incident and diffracted rays there is no significant improvement.

Design and focal properties: Rowland-circle mounting

The only degrees of freedom that are available when designing a single-beam interference grating are the coordinates of the center of curvature of the convex spherical mirror. These may conveniently be expressed in polar form as L and θ, where L is the distance from the pole of the grating to the center of curvature and θ is the angle between the radius of the blank and the line joining the pole to the point (Figure 3).

The pitch of the grating is given by

$$d = \frac{\lambda o}{2\sin\theta}$$

If we specify d, then θ is fixed and our only variable is L.

If $L = R\cos\theta$, where R is the radius of the blank, then the center of curvature of the mirror lies on the Rowland circle, and the focal curve of the grating will be the Rowland circle. Since the grooves are curved, the image-forming properties will be different from those of a conventional ruled grating, but the position of the spectral images will be the same.

Calculating astigmatism in the Eagle mounting for a classical and a single-beam concave grating made with light at 458nm, we see that at 458nm the image is perfect, and that at other wavelengths the image of the single-beam grating is superior.

Non-Rowland circle mounting

We now consider whether it is possible, by a suitable choice of L, our remaining degree of freedom, to design a grating where the focal distance is constant.

By substituting mirrors of various radii of curvature for the convex mirror in Figure 3, we can produce a series of gratings corresponding to various values of L. The focal curves for such a series of gratings with 1200gr/mm on blanks of various radii is shown in Figure 5. The curve of particular interest is that corresponding to a value of L of 225mm (by theory it should have been 220mm).

For this grating the focal distance is the same at 458mm in first order,

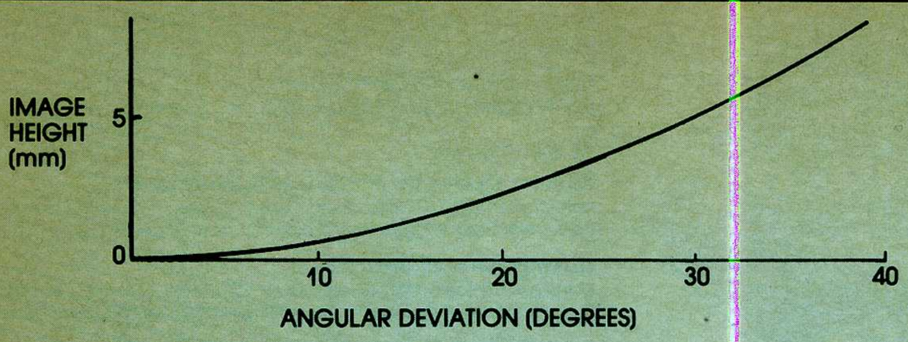

Figure 8. *A plot of the astigmatism at 458nm as a function of angular separation of incident and diffracted beams.*

and at all wavelengths in zero order. From a mathematical point of view, zero order corresponds to a wavelength of zero in the first (or any other) order. We may therefore argue that if there exists a value of L that gives the same focal distance for all wavelengths then that focal distance must apply to zero wavelength. That value must therefore be equal to the radius of curvature of the blank, since this is the focal distance in zero order. (N.B. Focal distance in this context means the distance between the grating and the point where the image and source are superimposed. It should not be confused with focal length.)

It is clear from Figure 5 that even with a slight mismatch of mirror radius the focal distance remains virtually constant for the spectral range between 350nm and 700nm. We can therefore conclude that it is indeed possible to produce a grating that will maintain focus as it is rotated.

This may therefore be used as the basis of a very simple spectrometer as depicted in Figure 6. This is similar to the Seya-Namioka mounting in that it requires only a fixed entrance and exit slit and is scanned by a simple rotation of the grating. However, the angle between the incident and diffracted beams is close to zero, whereas with Seya-Namioka it is approximately 65°. The instrument is therefore more compact, which in many spectroscopic applications can itself be a significant practical advantage.

Image quality

Given that we can produce a grating where the image is formed in a convenient position, we must now consider the quality of that image. The most significant parameter is likely to be that of astigmatism, which falls to zero at the wavelength of manufacture. The length of the astigmatic image at other wavelengths (or the size of any aberration) will depend upon the dimensions and numerical aperture of the grating.

In Figure 7 we plot the astigmatism for some wavelengths between 350nm and 700nm for a 1200gr/mm grating on a 220nm-radius blank and an aperture of 35mm in diameter. It is instructive to compare this result with that of a two-beam concave grating corrected for use at an included angle of just over 60°. In this comparison both of the gratings were tested under the conditions for which they were intended to be used. The gratings were chosen as far as possible to be equivalent, and it would appear that the single-beam concave grating has a slightly superior performance as one departs from the ideal wavelength.

For completeness we show the performance of the single-beam concave grating when used in the configuration for which the two-beam concave interference grating was designed and the astigmatism when the two-beam type was used in the Littrow mounting. This emphasizes the fact that the two are not really compatible. The data indicates that the single-beam type in a Littrow mount is ideal for use as a scanning monochromator, where the wavelength selection is accomplished by a simple rotation of the grating.

The measurements of astigmatism for the single-beam grating were made in the true Littrow condition using a beamsplitter to separate the incident and returning beams. In any practical arrangement it would be necessary to separate the entrance and exit slits, so there would be a finite angle between the beams. As we depart from the ideal Littrow condition we introduce astigmatism.

In Figure 8 we plot the astigmatism at 458nm (the wavelength of construction) as a function of angular separation of the incident and diffracted beams. From this we can see that it is quite feasible to introduce sufficient slit separation to accommodate a detector without introducing significant astigmatism. For special applications, such as in-line use, folding mirrors may also be used.

There is a great deal of interest in the use of a grating spectrograph, allowing data to be extracted quickly by use of a detector array. The optimization of L for this use is under investigation, and preliminary results indicate good performance at the moderate resolution provided by use with newly developed larger-element detector arrays.

Concave gratings have benefited from several developments in grating technology. The use of laser-generated holographic techniques to produce the grating grooves yields both lower stray light and new design freedom. Control of the positioning points for two generating beams permits corrections, reducing the aberrations inherent in a ruled version. These gratings, referred to as two-beam interference gratings, have been available for scanning use in a Seya-Namioka mount from several vendors in recent years.

Using developments from the National Physical Laboratory in England, the Optometrics Group first made available blazed UV holographic gratings, and has now incorporated this technique in a method of making a concave grating using standing waves from a single laser beam. The fact that the blazed grating achieves aberration correction in the extremely compact Littrow mount makes possible some unique advantages over ruled gratings and even over two-beam interference types. □

Reference

1. Hutley, M.C. (1982). *Diffraction Gratings.* Academic Press, New York.

Meet the author

Jay Zakrzewski is sales manager of PTR Optics Corp. of Waltham, Mass., one of the two companies that make up the Optometrics Group; the other is Optometrics Ltd. of Leeds, England. This article introduces the single-beam interference technique developed at the National Physical Laboratory in England.