

Introduction to reflective aberration corrected holographic diffraction gratings

By Steve Slutter, Wu Jiang, and Olivier Nicolle

The reflective diffraction grating is the heart of most spectroscopy systems today. Before the 1950's, the prism was the primary dispersive element in spectrometer designs. The use of an epoxy replication process in the 1950's led to the mass production of plane ruled reflective diffraction gratings. New availability of ruled gratings displaced the prism as the dispersive element of choice. The next advance in dispersive element development came with the development of the laser. The laser provided an alternative method to manufacture diffraction gratings. This process called "holography," was used to produce a sinusoidal groove pattern on a glass substrate that had significant performance advantages over its ruled grating counterpart. Further advances in the holographic manufacturing process have made custom groove profiles and groove shapes possible. Control of the grating groove shape makes aberration correction possible. This new design parameter has made possible a new class of instrument designs, aberration corrected concave grating designs.

Some of the first corrected designs were applied to concave gratings at Jobin Yvon in Longjumeau, France in 1969. At that time, they made concave gratings with astigmatism correction for the VUV (10 nanometer - 200 nanometer range) wavelength range. Concave optics are often used in the VUV to minimize instrument losses. The correction of aberrations, namely coma, spherical aberration, astigmatism and field curvature, made concave gratings available for the VUV, visible and infrared spectroscopy markets.

Holographic gratings have some significant advantages over ruled gratings. The most important advantage is reduced surface roughness. Reduced surface roughness decreases grating scatter and can improve detection limits. Raman Spectroscopy is one scientific method that took advantage of holographic gratings. The lower straylight, possible with holographic gratings, have improved the quality and accuracy of spectroscopic results.

The concave aberration corrected grating

The performance of spectrometers and spectrographs is judged by system resolution, throughput, and system limit of detection. These criteria involve grating efficiency, system light collection capability, system straylight and design aberrations. The use of holographic concave aberration corrected gratings allows optimization of all these parameters with a single optic. Each of these design criteria is described.

1) Grating efficiency: Holographic gratings are available in three different groove profiles. Each of these profiles has different efficiency advantages. Figures 1, 2, and 3 show the sinusoidal, laminar and a triangular groove profile respectively. The sinusoidal profile has the broadest spectral range of the three profiles. The maximum theoretical average efficiency (of unpolarized light) of the sinusoidal grating profile is 33.8%. Laminar and triangular groove profiles are produced with an Ion Etching process that shapes the groove profile. The laminar profile grating improves the efficiency, but the main advantage of this profile is the reduction in second order efficiency. The second order is reduced to as low as 0.4%. Applications in the VUV benefit because second order filters do not exist in this wavelength range. The triangular groove profile has efficiency profiles similar to ruled gratings. Peak efficiencies of 50% to 80% are common.

High groove density gratings can have efficiencies as high as 95% for a particular polarization. This is true for any of the groove profiles discussed above.

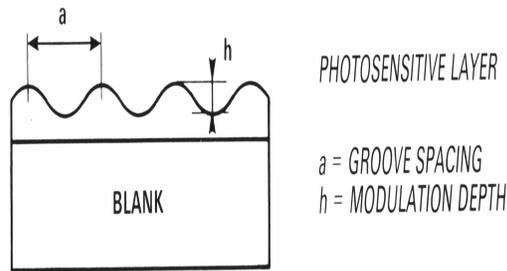


Figure 1. Sinusoidal groove profile.

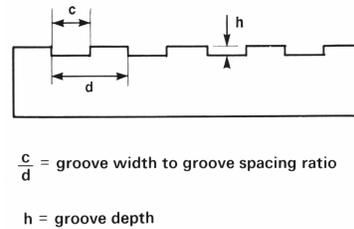


Figure 2. Lamellar groove profile.

α = Blaze angle

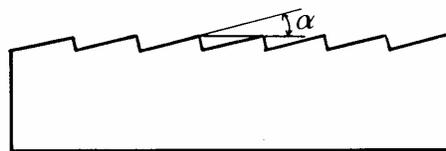


Figure 3. Triangular groove profile.

2) System light collection capability

Concave aberration corrected grating instruments are defined by the grating. Concave gratings are defined by their arm lengths and included angle. The grating is the sole optical element in a concave grating design. The light collection is determined by the f-number of the grating. F-number is the ratio of the grating focal length divided by the grating diameter (clear aperture). Aberration correction (discussed later in this paper) allows higher f-number collection as compared with the commercial spectrometer and spectrograph designs. Concave grating *spectrograph* designs with f-numbers of $f/2$ and faster (toward $f/1.5$) are common. Concave grating *spectrometer* designs with f-numbers of $f/2.5$ are practical. By comparison, most retail instruments use plane grating designs and operate at f-numbers between $f/3$ and $f/10$. Aberration correction allows designs to operate at high f-numbers because of reductions in the effects of aberrations (more on this topic later). High f-number designs, possible with concave grating designs, offer the advantage of increased light collection capability over plane grating designs. Light collection capability comparisons of instruments can be done by taking the ratio of the squares of the design f-numbers. To compare the collection ability of a $f/5$ plane grating design instrument and a $f/2$ concave grating design, calculate the ratio of 5^2 to 2^2 . The results of this calculation show a ratio of 25 to 4. The light collection of the $f/2$ concave grating design is more than six times greater than the $f/5$ design.

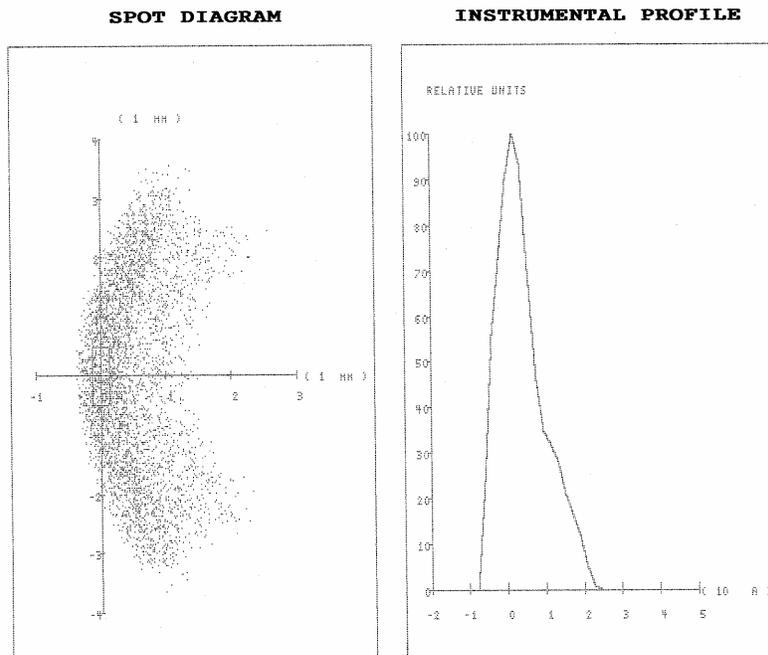
The system collection efficiency is optimized with concave gratings while providing a simple, cost-effective design. Additional mirrors and mirror mounts are not necessary in concave aberration corrected grating designs.

3) System straylight parameters

The process of manufacturing holographic gratings makes the grating surface smoother than ruled gratings. Surface roughness is the primary source of grating generated straylight. It is important to remember that everything scatters light. All gratings exhibit some amount of scattered light. The inherent lower scatter of holographic gratings has affected the system performance. Concave grating designs have two additional design advantages, with respect to system straylight, over most commercial plane grating designs. First, grating scatter in Czerny Turner and Fastie Ebert designs is collected and focussed, by the focussing mirror, toward the exit port. In concave grating designs the grating does not focus its own scattered light into the focal plane. Secondly, another form of system straylight is rediffracted light. Rediffracted light is light that is diffracted by the grating and redirected back to the grating a second time (unintentionally of course). When other concave optics (collimating and focussing mirrors) are used in an instrument design it is more likely that light may be rediffracted. Careful design effort is necessary to prevent rediffracted light. Concave gratings are immune from this problem when working at f-numbers greater than $f/2$ with low groove density (<600 grooves per millimeter/mm) gratings.

4) Aberration correction

Aberration correction is the most important benefit of concave aberration corrected holographic gratings. To understand the benefit of aberration correction it is important to understand the main aberrations in spectrometer and spectrograph designs and their impact on system results.



BANDPASS (FWHM) = 11.5 ANGSTROMS
TH = 18.0 P.C.
MAGNIFICATION Y = 2.69
MAGNIFICATION Z = -0.940
DISPERSION = 15.35 ANGSTROMS / MM

Figure 4. Exit plane image showing aberration effects.

Figure 4 shows the focal plane image of a 200 micron, 1mm high input slit. Consider the effect of this image on a 1mm high detector (whether it is an array pixel or an exit slit).

The effects of coma, astigmatism and spherical aberration are plainly visible in Figure 4. The exit slit image has “grown” in height by approximately 7mm. This effect is astigmatism. The width of the exit slit image is appreciably wider and fades off in intensity to one side. This effect is coma. The blurry, defocused property of the entire image is spherical aberration. The last major instrument aberration, field curvature, can be observed as the curve of this output image. These aberrations, left unaddressed can cause a degradation of the system performance.

The effects of coma, spherical aberration, astigmatism and field curvature are well understood for lenses, but their effect on spectroscopic measurements is not always well understood. Some description is necessary for how these aberrations relate to the exit focal plane of a spectrometer or spectrograph¹⁻².

Coma is an aberration resulting from using off axis optics. Coma causes an unsymmetrical spectral line broadening. This broadening leads to resolution losses and straylight. On a detector array, the impact is pixel to pixel crosstalk and loss of resolution. Coma can be corrected in some instruments, at one wavelength, by adjusting the optical geometry.¹ Coma can be corrected at many wavelengths in the concave aberration corrected grating design.

Astigmatism (AST) is another aberration resulting from the use of off axis optics. Point sources “grow” in height as the longitudinal astigmatism increases. Longitudinal astigmatism is the result of off axis rays separating into tangential and sagittal components². Astigmatism effects can lead to a 400-micron input fiber (at the input slit position) “grow” to 2 millimeters high at the output focal plane. When using a 0.5 millimeters high array, and the exit focal plane image is 2 millimeters, 75% of the output signal is not measured. This effect leads to loss of system throughput and detectability. Astigmatism is corrected in plane grating instruments using aspheric optics. Toroidal mirrors are often used to reduce astigmatism for inputs on the optical axis. Astigmatism is corrected over wide spectral ranges with corrected gratings.

Spherical aberration (SA) is a consequence of using spherical mirrors. A spherical mirror does not precisely focus a point to a point. As light rays move further away from the center axis of a mirror, the focal point moves closer to the mirror. A zone of confusion is created in the image plane² because of the changing focal point with distance from center axis. This “zone” of confusion prevents the ability to obtain a sharp focussed image (see recommended reading #2). SA is difficult to eliminate without the use of aspheric optics. The result of SA is loss of resolution. Imaging performance degrades causing crosstalk from adjacent wavelengths. Parabolic mirrors are used in some designs to correct SA. In aberration corrected designs the grating is designed to correct SA. SA increases as the f-number increases (toward f/1). High aperture spectrographs (f/1.7) performance would be unusable without correction of SA. Reduced SA can improve the resolution capability allowing for smaller slits. *Field curvature* (FC) is the shape of the image plane (usually called the Petzel Field). The shape of the field determines the shape of images at the exit. Field curvature can cause calibration errors for off axis sources and pixel to pixel crosstalk on arrays. Calibration errors and increased blur, of off axis inputs, are considered straylight.

¹A. Shafer, L. Megill, L. Droppelman, “Aberrations in spectrometers,” J. Opt. Soc. Am, 54, 879, 887 (1964).

²J. Lerner and A. Thevenon, “The Optics of Spectroscopy,” a tutorial from ISA, Vol. 2 1988.

Aberration corrected gratings can change the shape of the exit focal plane field. Aberration corrected gratings are often called “flat field” gratings. This feature prevents image degradation for off axis images. Designs without this correction often suffer from spatial and spectral resolution losses for off axis inputs.

Coma, SA, and FC contribute to near end straylight (light from adjacent wavelengths). Light that does not properly strike the detector decreases the system performance. The signal to noise ratio suffers because of low throughput per pixel and increased pixel to pixel crosstalk.

Advantage review

Putting the advantages of efficiency, system light collection capability, system straylight advantages and aberration correction together provides a clear view of the advantages of the holographic concave aberration corrected grating designs. The performance advantages of aberration corrected concave gratings, together with the simple, straightforward design will optimize the system performance.

To illustrate the possibilities of concave aberration corrected grating designs, figures 5 and 6 show the performance of two concave aberration corrected grating designs.

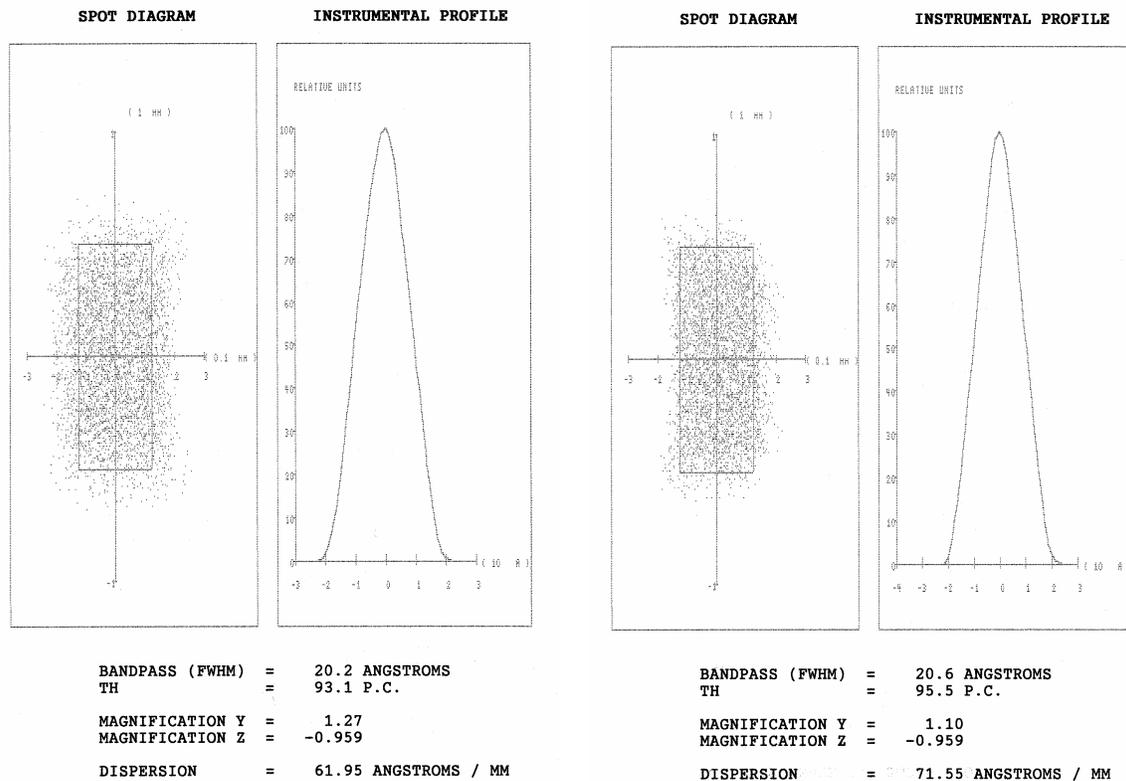


Figure 5. ISA H1034 scanning spectrometer spot diagrams

Figure 5 shows spot diagrams of the ISA H1034, 100-millimeter focal length, scanning spectrometer. This instrument uses 1200 grooves per millimeter concave aberration corrected $f/3$ grating. The 250 nanometer to 750-nanometer wavelength range is very well corrected for coma, SA, AST and field curvature. The spot

diagrams agree well with actual data taken on the instrument. Note that the resolution is almost identical across the wavelength range. The image size is also well maintained throughout the usable range of the instrument. Figure 6 shows spot diagrams of an ISA SF100 spectrograph. This is a $f/2$, 100-millimeter focal length instrument. These spot diagrams are for nine 100μ fibers with 250μ separation. Good spatial resolution is obtained in both the spectral and spatial directions. Note the separation of the fiber inputs for on axis and off axis inputs.

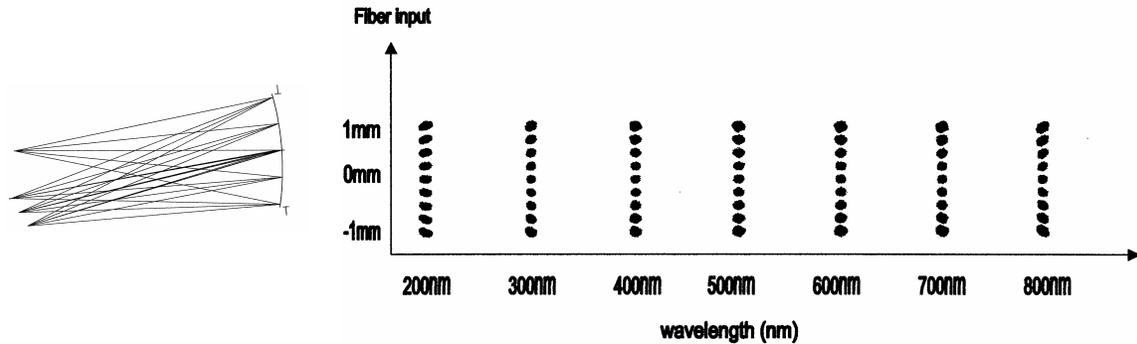


Figure 6. System layout and spit diagrams for ISA SF100 spectrograph.

Technology pushing instrument design

In the past three decades detector technology has progressed from film to phototubes to photodiode arrays to charge coupled devices (CCD's). The spectrometer and spectrograph designs have had to keep up. The use of small diameter optical fibers (with high numerical apertures) coupled with new detector technology have made improved imaging of existing instruments much more important. Good *off axis* performance has become necessary as applications using fiber arrays and tall CCD's arrays are used together in applications. It is in this area that aberration corrected holographic grating designs have made the biggest impact. Aberrations such as coma, spherical aberration, astigmatism and field make point to point imaging a difficult challenge. Many instrument companies have taken the route of using expensive aspherical optics or pre-optics to improve imaging of existing plane grating designs. They have been partially successful. Few commercial designs completely couple the full f-number of an optical fiber. Concave aberration corrected grating designs have met this challenge and won.

Commercially available instruments are designed as all-purpose instruments. They must adapt to applications that work well in the VUV through the far Infrared in scanning and image modes. For dedicated applications, a more focussed design can lead to an instrument that outperforms the all-purpose, one size fits all, instrument design. For those users with dedicated, repetitive applications (as with most OEM grating customers), concave gratings are the obvious choice.

As a side note, aberration correction is not limited to concave surfaces. In 1987, a Jobin Yvon HR640 (a 0.64m single Czerny Turner design) was manufactured using an aberration corrected plane grating¹. This instruments achieve near diffraction limited resolution at its design wavelength. This nearly symmetrical Czerny Turner spectrometer benefited greatly by the elimination of AST, SA, and Coma.

Another advantage of aberration correction gratings well worth mentioning, is the ability to correct for aberrations in other parts of the optical train. Other system aberrations (e.g., aberrations from lenses, mirrors or sample-related problems) can be corrected with an appropriate grating design. The grating design can incorporate the required correction to correct for system coma, spherical aberration, astigmatism and field curvature. This system design approach can improve resolution and spatial imaging.

**Ruled or Holographic
Plane Ruled versus Concave Holographic
When and Why?**

Given all of the advantages of concave aberration corrected gratings, one might ask: why are plane-ruled gratings (or plane holographic gratings for that matter) still used if concave aberration corrected gratings are so great? To answer this question, first let us separate the ruled parameter from the plane (flat) aspect.

Ruled gratings have two occasions where they are the gratings of choice. They are:

- 1) Groove densities coarser than 50 grooves per millimeter. Holographic gratings are exceedingly difficult to manufacture at this coarse groove density. This groove density is often used in infrared applications. Ruled gratings have a wide variety of existing infrared blazed gratings. Holographic grating limitations are related to groove spacing and groove depth.
- 2) When the application requires work in higher orders (e.g., 100th order) coarse gratings called Echelle gratings are used. The groove profile of the Echelle is not possible with the holographic process.

The (flat ruled or holographic) aspects. Many instruments use plane-grating designs because of flexibility. Designs like the Czerny Turner layout maintain resolution over a wide range of grating rotation (excluding the effects of coma and field curvature). A Czerny Turner design, with the appropriate choice of grating (and mirror coatings), can operate in the 50-nanometer to 50-micron wavelength range (50 grooves per millimeter to 3600 grooves per millimeter). The design can operate as a spectrometer or as a spectrograph. The “all purpose instruments” are ideal if your work includes changing needs of spectral ranges and dispersion.

Applications with fixed spectral ranges, not requiring the need to change gratings, can benefit from the simplicity, cost advantages, and performance of a concave aberration corrected grating design. Concave aberration corrected grating designs are optimized to perform well over a specific wavelength range. Working outside the designed working range will compromise performance.

As a research tool, plane grating designs offer more flexibility including multiple gratings (on turrets), multiple inputs and outputs, and multiple detectors. As a dedicated application device, the concave aberration corrected grating design is usually the best choice.

In considering the question of when to use ruled plane gratings or plane holographic gratings, the answer is simple. Use a holographic grating whenever it is available. When considering the question of when to use plane versus concave the answer is also simple. A concave grating should be used in instrument designs that are dedicated to one spectral range and one basic function. An example of this type of design would be a single input spectrograph operating with an one inch long array covering the 350-nanometer to 1000-nanometer wavelength range. Whenever simplicity, cost, and performance are important, the concave option should be explored.

Holographic, concave, aberration corrected grating designs offer many advantages to spectrograph and

spectrometer users. With the use of optical analysis design tools, aberration corrected gratings can be designed to correct instrument and system aberrations. This design parameter offers many advantages to instrument and system designers.

Table 1 lists some advantages of holographic, aberration corrected, concave grating designs.

Table 1

Advantages of holographic aberration corrected, concave, grating designs

Advantage	Benefit
Aberration correction	Improved resolution, imaging, calibration
High f-number	Maximum light collection, improved system performance
Simplicity	No additional mounts, mirrors, or other optics required
No rediffracted light	Light focussed back to the grating is easily avoidable
Low straylight	The holographic process has less scatter than ruled gratings
Flat efficiency curve	Allows for a broad wavelength range
Gratings for VUV-IR	Gratings available for 10nm-10microns
Groove densities up to 6000gv/mm	Far exceeds ruled grating capability
Sizes up to 600mm diameter	Far exceeds ruled grating capability

Conclusion

Design success will often depend on achieving the optimal coupling of all of the system components. Aberration corrected, holographic grating designs are used in systems to optimize the throughput while reducing noise. Using a concave, aberration corrected, blazed, holographic grating will increase the chances of meeting the most difficult spectrometer/spectrograph design targets. The convenience, simplicity, and effectiveness have made concave aberration corrected grating designs a common tool in a wide range of markets. Some of these markets include colorimetry, biotechnology, semiconductor, telecommunications, and analytical chemistry.

As applications become more demanding and detector technology evolves, the need for aberration correction grating designs will play an increasingly important role in spectroscopy. We are already seeing detector sizes shrink and dynamic ranges grow. Designs of new analytical instruments have begun to take full advantages of the capabilities of the concave holographic gratings.