THE OPTICS OF SPECTROSCOPY

A TUTORIAL By J.M. Lerner and A. Thevenon

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Section 1: Diffraction Gratings - Ruled & Holographic

Diffraction gratings are manufactured either classically with the use of a ruling engine by burnishing grooves with a diamond stylus or holographically with the use of interference fringes generated at the intersection of two laser beams. (For more details see Diffraction Gratings Ruled & Holographic Handbook, Reference 1.)

Classically ruled gratings may be plano or concave and possess grooves each parallel with the next. Holographic grating grooves may be either parallel or of unequal distribution in order that system performance may be optimized. Holographic gratings are generated on plano, spherical, toroidal, and many other surfaces.

Regardless of the shape of the surface or whether classically ruled or holographic, the text that follows is equally applicable to each. Where there are differences, these are explained.

1.1 Basic Equations
Before introducing the basic equations, a brief note on monochromatic light and continuous spectra must first be considered.

Monochromatic light has infinitely narrow spectral width. Good sources which approximate such light include single mode lasers and very low pressure, cooled spectral calibration lamps. These are also variously known as "line" or "discrete line" sources.

A continuous spectrum has finite spectral width, e.g. "white light". In principle all wavelengths are present, but in practice a "continuum" is almost always a segment of a spectrum. Sometimes a continuous spectral segment may be only a few parts of a nanometer wide and resemble a line spectrum.

The equations that follow are for systems in air where $\mu_0 = 1$. Therefore,$\lambda = \lambda_0$ = wavelength in air.

Definitions Units

alpha - angle of incidence degrees
beta - angle of diffraction degrees
k - diffraction order integer
n - groove density grooves/mm
D_V - the included angle degrees (or deviation angle)
μ_0 - refractive index
λ - wavelength in vacuum nanometers (nary)
λ_0 - wavelength in medium of refractive index, μ_0, where $\lambda_0 = \lambda m_0$
1 nm = 10^{-6} mm; 1 micrometer = 10^{-3} mm; 1 A = 10^{-7} mm

The most fundamental grating equation is given by:

$$\sin \alpha + \sin \beta = 10^{-6} kn\lambda \quad (1\text{-}1)$$

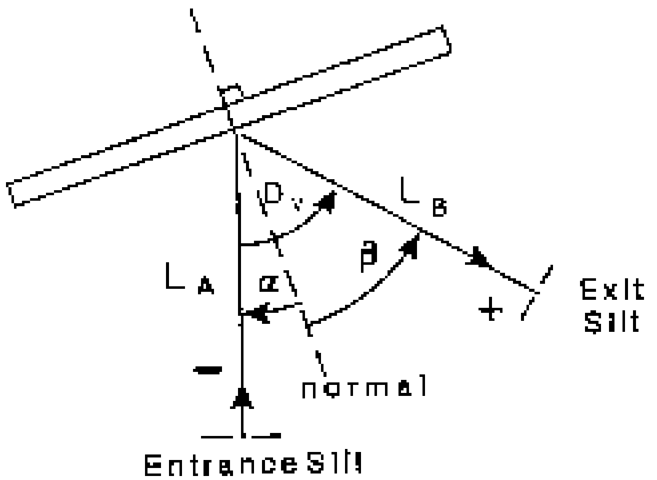
In most monochromators the location of the entrance and exit slits are fixed and the grating rotates around a plane through the center of its face. The angle, Dv, is, therefore, a constant determined by:

$$D_V = \beta - \alpha \qquad (1\text{-}2)$$

If the value of alpha and beta is to be determined for a given wavelength, lambda, the grating equation (1-1) may be expressed as:

$$10^{-6}\, kn\lambda = 2 \sin\left[\frac{(\beta+\alpha)}{2}\right] \cos\left[\frac{(\beta-\alpha)}{2}\right] \qquad (1\text{-}3)$$

Assuming the value Equations (1-2) and (1-3). See Figs. 1 and 2 and Section 2.6.



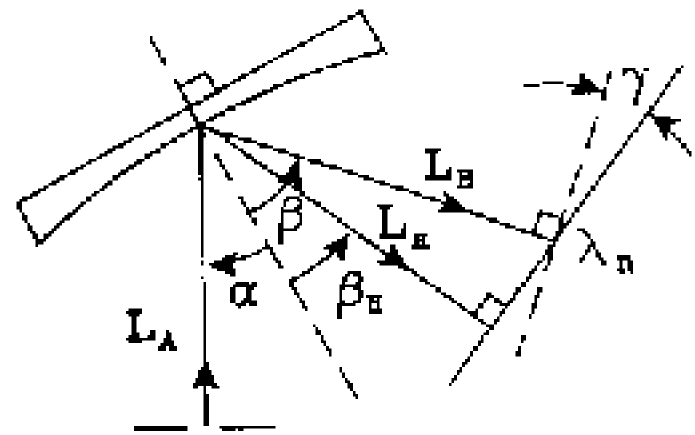


Figure 1 - Monochromator Configuration Figure 2 - Spectrograph Configuration

L_A = Entrance arm length

L_B = Exit arm length

$beta_H$ = Angle between the perpendicular to the spectral plane and the grating normal

L_H = Perpendicular distance from the spectral plane to grating

Table 1 shows how alpha and beta vary depending on the deviation angle for a 1200 g/mm grating set to diffract 500 nm in a monochromator geometry based on Fig. 1.

Table 1: Variation of Incidence, alpha, and Angle of Diffraction, beta, with Deviation Angle, Dv, at 500 nm in First Order with 1200 g/mm Grating

Deviation	alpha	beta
0	17.458	17.458 (Littrow)
10	12.526	22.526
20	7.736	27.736
24	5.861	29.861
30	3.094	33.094

40	-1.382	38.618
50	-5.670	44.330

1.2 Angular Dispersion

$$\frac{d\beta}{d\lambda} = \frac{kn\ 10^{-6}}{\cos\ \beta} \quad (1\text{-}4)$$

dbeta- angular separation between two wavelengths (radians)

dlamda - differential separation between two wavelengths nm

1.3 Linear Dispersion

Linear dispersion defines the extent to which a spectral interval is spread out across the focal field of a spectrometer and is expressed in nm/mm, °A/mm, cm^{-1}/mm, etc. For example, consider two spectrometers: one instrument disperses a 0.1 nm spectral segment over 1 mm while the other takes a 10 nm spectral segment and spreads it over 1 mm.

It is easy to imagine that fine spectral detail would be more easily identified in the first instrument than the second. The second instrument demonstrates "low" dispersion compared to the "higher" dispersion of the first. Linear dispersion is associated with an instrument's ability to resolve fine spectral detail.

Linear dispersion perpendicular to the diffracted beam at a central wavelength, A, is given by:

$$\frac{d\lambda}{dx} = \frac{10^{6}\ \cos\ \beta}{kn\ L_B} \quad (1\text{-}5)$$

where L_B is the effective exit focal length in mm and dx is the unit interval in mm. See Fig. 1.

In a monochromator, L_B is the arm length from the focusing mirror to the exit slit or if the grating is concave, from the grating to the exit slit. Linear dispersion, therefore, varies directly with cos beta, and inversely with the exit path length, L_B, order, k, and groove density, n.

In a spectrograph, the linear dispersion for any wavelength other than that wavelength which is normal to the spectral plane will be modified by the cosine of the angle of inclination (gamma) at wavelength Lambda_n. Fig. 2 shows a "flat field" spectrograph as used with a linear diode array.

Linear Dispersion

$$\frac{d\lambda_n}{dx} = \frac{10^{6}\ \cos\ \beta\ \cos\ \gamma}{kn\ L_{B_{\lambda n}}} \quad (1\text{-}6)$$

$$\gamma \simeq \beta_H - \beta \quad (1\text{-}7)$$

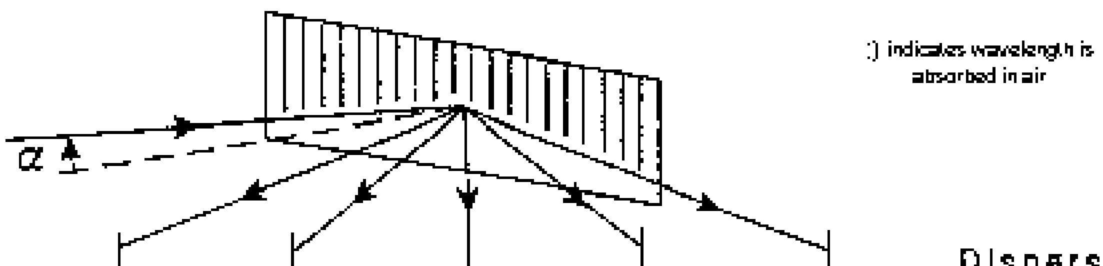
$$\frac{d\lambda_n}{dx} = \frac{10^6 \cos\beta \cos^2\gamma}{kn\, L_H} \quad (1\text{-}8)$$

1.4 Wavelength and Order

Figure 3 shows a first order spectrum from 200 to 1000 nm spread over a focal field in spectrograph configuration. From Equation (1-1) with a grating of given groove density and for a given value of alpha and beta:

$$k\lambda = \text{constant} \quad (l\text{-}9)$$

so that if the diffraction order k is doubled, lambda is halved, etc.



Order						Dispersion at Central Wavelength
1st	200	400	600	800	1000	10 nm/mm
2nd	(100)	200	300	400	500	5
3rd	(66.6)	(133.3)	200	266.6	333.3	3.3
4th	(50)	(100)	(150)	200	250	2.5

Figure 3 - Dispersion and Order

If, for example, a light source emits a continuum of wavelengths from 20 nm to 1000 nm, then at the physical location of 800 nm in first order (Fig. 3) wavelengths of 400, 266.6, and 200 nm will also be present and available to the same detector. In order to monitor only light at 800 nm, filters must be used to eliminate the higher orders.

First order wavelengths between 200 and 380 nm may be monitored without filters because wavelengths below 190 nm are absorbed by air. If, however, the instrument is evacuated or N_2 purged, higher order filters would again be required.

1.5 Resolving "Power"

Resolving "power" is a theoretical concept and is given by

$$R = \frac{\lambda}{d\lambda} \quad \text{(dimensionless) (1-10)}$$

where, dlambda is the difference in wavelength between two spectral lines of equal intensity. Resolution is then the ability of the instrument to separate adjacent spectral lines. Two peaks are considered resolved if the distance between them is such that the maximum of one falls on the first minimum of the other. This is called the Rayleigh criterion.

It may be shown that:

$$R = \frac{\lambda}{d\lambda} = k\ n\ W_g = kN \quad (1\text{-}11)$$

lambda - the central wavelength of the spectral line to be resolved

Wg - the illuminated width of the grating

N - the total number of grooves on the grating

The numerical resolving power "R" should not be confused with the resolution or bandpass of an instrument system (See Section 2).

Theoretically, a 1200 g/mm grating with a width of 110 mm that is used in first order has a numerical resolving power R = 1200 x 110 = 132,000. Therefore, at 500 nm, the bandpass

$$d\lambda = \frac{500}{132{,}000} = 0.0038\ \text{nm}$$

In a real instrument, however, the geometry of use is fixed by Equation (1-1). Solving for k:

$$k = \frac{\sin\alpha + \sin\beta}{10^{-6}\ n\ \lambda} \quad (1\text{-}12)$$

But the ruled width, Wg, of the grating:

$$W_g = \frac{N}{n} \qquad \text{then } N = W_g\ n \quad (1\text{-}13)$$

where $\frac{1}{n} = \text{mm/groove}$ (1-14)

after substitution of (1-12) and (1-13) in (1-11).

Resolving power may also be expressed as:

$$R = W_g \frac{(\sin\alpha + \sin\beta)}{10^{-6}\lambda} \quad (1\text{-}15)$$

Consequently, the resolving power of a grating is dependent on:

* The width of the grating

* The center wavelength to be resolved

* The geometry of the use conditions

Because bandpass is also determined by the slit width of the spectrometer and residual system aberrations, an achieved bandpass at this level is only possible in diffraction limited instruments assuming an unlikely 100% of theoretical. See Section 2 for further discussion.

1.6 Blazed Gratings

Blaze: The concentration of a limited region of the spectrum into any order other than the zero order. Blazed gratings are manufactured to produce maximum efficiency at designated wavelengths. A grating may, therefore, be described as "blazed at 250 nm" or "blazed at 1 micron" etc. by appropriate selection of groove geometry.

A blazed grating is one in which the grooves of the diffraction grating are controlled to form right triangles with a "blaze angle, w," as shown in Fig. 4. However, apex angles up to 110° may be present especially in blazed holographic gratings. The selection of the peak angle of the triangular groove offers opportunity to optimize the overall efficiency profile of the grating.

1.6.1 Littrow Condition

Blazed grating groove profiles are calculated for the Littrow condition where the incident and diffracted rays are in autocollimation (i.e., alpha = beta). The input and output rays, therefore, propagate along the same axis. In this case at the "blaze" wavelength lambda$_B$.

$$\sin\alpha + \sin\beta = kn\,\lambda_B\,10^{-6}$$

$$\omega = \alpha = \beta \quad \text{where } \omega = \text{blaze angle.}$$

$$2\sin\omega = kn\,\lambda_B\,10^{-6} \quad (1\text{-}16)$$

For example, the blaze angle (w) for a 1200 g/mm grating blazed at 250 nm is 8.63° in first order (k = 1).

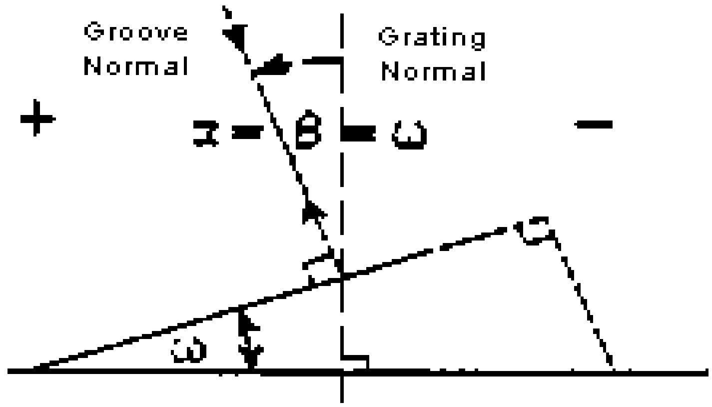


Figure 4 - Littrow Condition for a Single Groove of a Blazed Grating

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1.6.2 Efficiency Profiles

Unless otherwise indicated, the efficiency of a diffraction grating is measured in the Littrow configuration at a given wavelength.

% Absolute Efficiency = (energy out /energy in) X (100/1) (1-17)

% Relative Efficiency = (efficiency of the grating / efficiency of a mirror) X (100/1) (1-18)

Relative efficiency measurements require the mirror to be coated with the same material and used in the same angular configuration as the grating.

See Figs. 5a and 5b for typical efficiency curves of a blazed, ruled grating, and a non-blazed, holographic grating, respectively.

As a general approximation, for blazed gratings the strength of a signal is reduced by 50% at two-thirds the blaze wavelength, and 1.8 times the blaze wavelength.

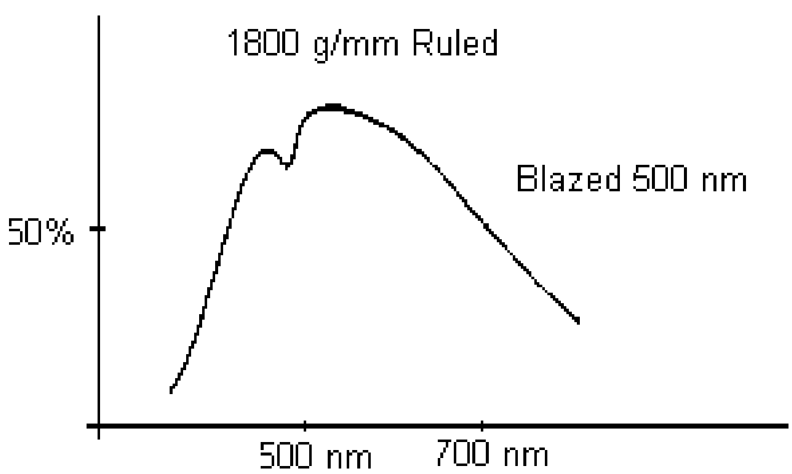

Figure 5a - Efficiency Curve of a Blazed, Ruled Grating

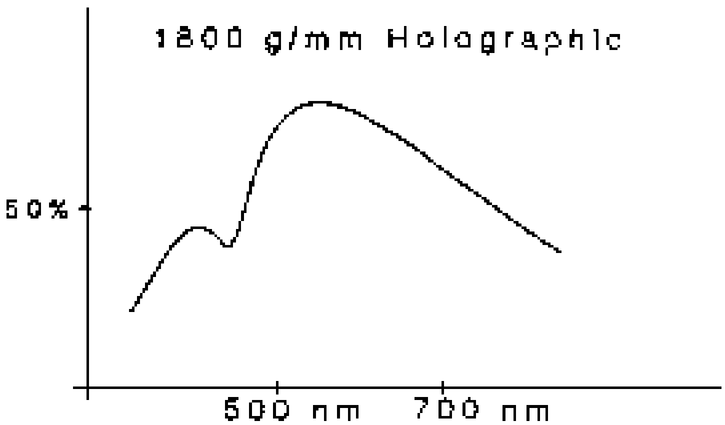

Figure 5b - Efficiency Curve of a Non-Blazed, Holographic Grating.

1.6.3 Efficiency and Order

*A grating blazed in first order is equally blazed in the higher orders Therefore, a grating blazed at 600 nm in first order is also blazed at 300 nm in second order and so on.

*Efficiency in higher orders usually follows the first order efficiency curve.

*For a grating blazed in first order the maximum efficiency for each of the subsequent higher orders decreases as the order k increases.

*The efficiency also decreases the further off-Littrow (alpha does not equal beta) the grating is used.

Holographic gratings may be designed with groove profiles that discriminate against high orders. This may be particularly effective in the VUV using laminar groove profiles created by ion-etching.

Note: Just because a grating is "non-blazed" does not necessarily mean that it is less efficient! See Fig. Sb showing the efficiency curve for an 1800 g/mm sinusoidal grooved holographic grating.

1.7 Diffraction Grating Stray Light

Light other than the wavelength of interest reaching a detector (often including one or more elements of "scattered light") is referred to as stray light.

1.7.1 Scattered Light

Scattered light may be produced by either of the following:

(a) Randomly scattered light due to surface imperfections on any optical surface.

(b) Focused stray light due to non-periodic errors in the ruling of grating grooves.

1.7.2 Ghosts

If the diffraction grating has periodic ruling errors, a ghost, which is not scattered light, will be focused in the dispersion plane. Ghost intensity is given by:

IG = IP n^2 k^2 e^2 pi^2 (l-l9)

where,

IG =ghost intensity

IP = parent intensity

n = groove density

k =order

e =error in the position of the grooves

- Ghosts are focused and imaged in the dispersion plane of the monochromator.
- Stray light of a holographic grating is usually up to a factor of ten times less than that of a classically ruled grating, typically nonfocused, and when present, radiates through 2pi steradians.
- Holographic gratings show no ghosts because there are no periodic ruling errors and, therefore, often represent the best solution to ghost problems.

1.8 Choice of Gratings

1.8.1 Uhen to Choose a Holographic Grating

(1) When grating is concave.
(2) When laser light is present, e.g., Raman, laser fluorescence, etc.
(3) Any time groove density should be 1200 g/mm or more (up to 6000 g/mm and 120 mm x 140 mm in size) for use in near UV , VIS, and near IR.
(4) When working in the W below 200 nm down to 3 nm.
(5) For high resolution when high groove density will be superior to a low groove density grating used in high order ($k > 1$).
(6) Whenever an ion-etched holographic grating is available.

1.8.2 When to Choose a Ruled Grating

(1) When working in IR above 1.2 um, if an ion-etched holographic grating is unavailable.
(2) When working with very low groove density, e.g., less than 600 g/mm.

Remember, ghosts and subsequent stray light intensity are proportional to the square of order and groove density (n^2 and k^2 from Equation (1-18)). Beware of using ruled gratings in high order or with high groove density.

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Section 2:Monochromators & Spectrographs

2.1 Basic Designs

Monochromator and spectrograph systems form an image of the entrance slit in the exit plane at the wavelengths present in the light source. There are numerous configurations by which this may be achieved -- only the most common are discussed in this document and includes Plane Grating Systems (PGS) and Aberration Corrected Holographic Grating (ACHG) systems.

Definitions

L_A - entrance arm length
L_B - exit arm length
h - height of entrance slit
h' - height of image of the entrance slit
alpha - angle of incidence
beta - angle of diffraction
w - width of entrance slit
w' - width of entrance slit image
Dg - diameter of a circular grating
Wg - width of a rectangular grating
Hg - height of a rectangular grating

2.2 Fastie-Ebert Configuration

A Fastie-Ebert instrument consists of one large spherical mirror and one plane diffraction grating (see Fig. 6).

A portion of the mirror first collimates the light which will fall upon the plane grating. A separate portion of the mirror then focuses the dispersed light from the grating into images of the entrance slit in the exit plane.

It is an inexpensive and commonly used design, but exhibits limited ability to maintain image quality off-axis due to system aberrations such as spherical aberration, coma, astigmatism, and a curved focal field.

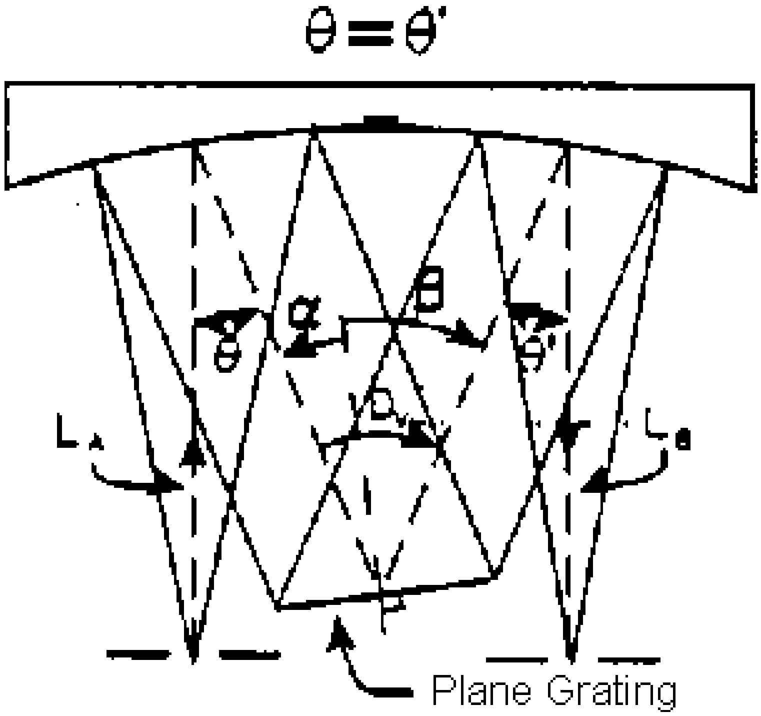


Figure 6 - Fastie-Ebert Configuration

2.3 Czerny-Turner Configuration
The Czerny-Turner (CZ) monochromator consists of two concave mirrors and one piano diffraction grating (see Fig. 7).

Although the two mirrors function in the same separate capacities as the single spherical mirror of. the Fastie-Ebert configuration, i.e., first collimating the light source (mirror 1), and second, focusing the dispersed light from the grating (mirror 2), the geometry of the mirrors in the Czerny-Turner configuration is flexible.

By using an asymmetrical geometry, a Czerny-Turner configuration may be designed to produce a flattened spectral field and good coma correction at one wavelength. Spherical aberration and astigmatism will remain at all wavelengths.

It is also possible to design a system that may accommodate very large optics.

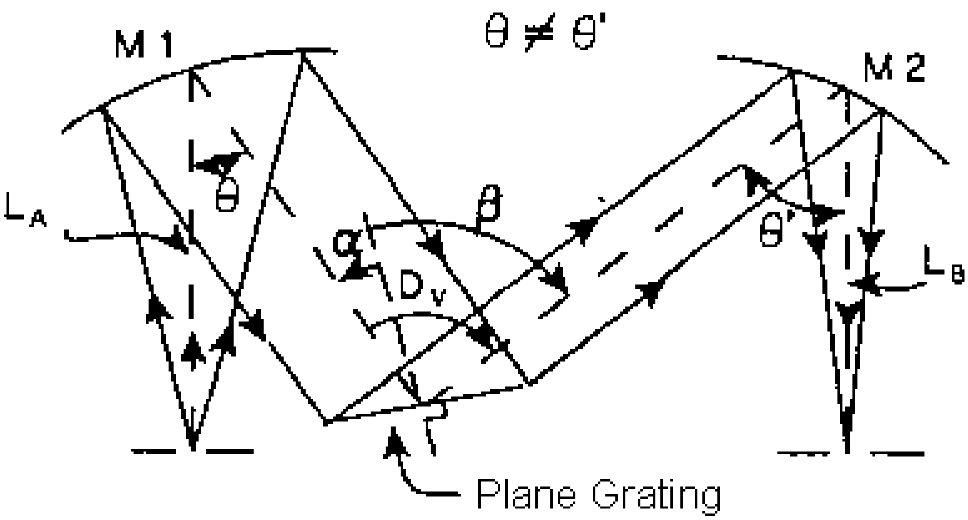


Figure 7 - Czerny-Turner Configuration

2.4 Czerny-Turner/Fastie-Ebert PGS Aberrations

PGS spectrometers exhibit certain aberrations that degrade spectral resolution, spatial resolution, or signal-to-noise ratio. The most significant are astigmatism, coma, spherical aberration and defocusing. PGS systems are used off-axis, so the aberrations will be different in each plane. It is not within the scope of this document to review the concepts and details of these aberrations, (reference 4) however, it is useful to understand the concept of Optical Path Difference (OPD) when considering the effects of aberrations.

Basically, an OPD is the difference between an actual wavefront produced and a "reference wavefront that would be obtained if there were no aberrations. This reference wavefront is a sphere centered at the image or a plane if the image is at infinity. For example:

1) Defocusing results in rays finding a focus outside the detector surface producing a blurred image that will degrade bandpass, spatial resolution, and optical signal-to-noise ratio. A good example could be the spherical wavefront illuminating mirror M1 in Fig. 7. Defocusing should not be a problem in a PGS monochromator used with a single exit slit and a PMT detector. However, in an uncorrected PGS there is field curvature that would display defocusing towards the ends of a planar linear diode array. Geometrically corrected CZ configurations such as that shown in Fig. 7 nearly eliminate the problem. The OPD due to defocusing varies as the square of the numerical aperture.

2) Coma is the result of the off-axis geometry of a PGS and is seen as a skewing of rays in the dispersion plane enlarging the base on one side of a spectral line as shown in Fig. 8. Coma may be responsible for both degraded bandpass and optical signal-to-noise ratio. The OPD due to coma varies as the cube of the numerical aperture. Coma may be corrected at one wavelength in a CZ by calculating an appropriate operating geometry as shown in Fig. 7.

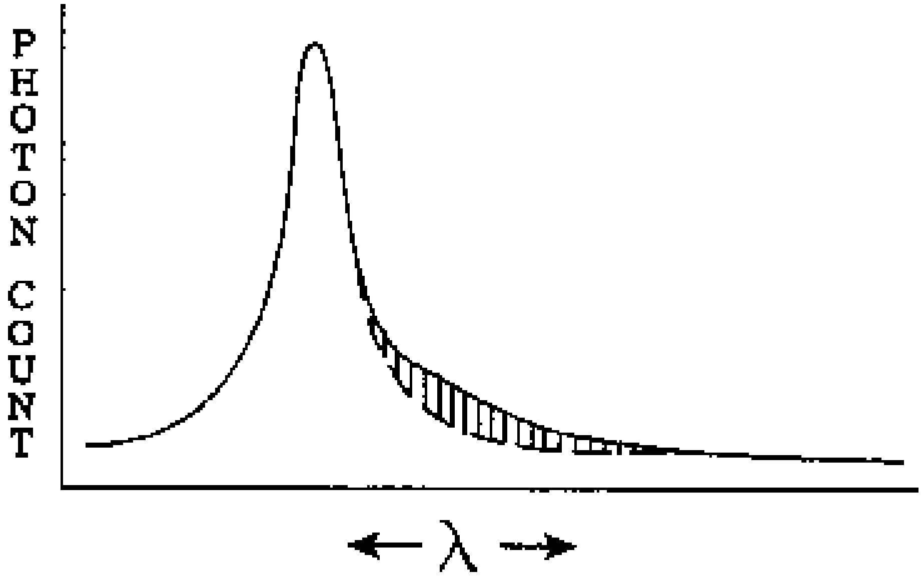


Figure 8 - The Effect of Coma

3) Spherical aberration is the result of rays emanating away from the center of an optical surface failing to find the same focal point as those from the center (See Fig. 9). The OPD due to spherical aberration varies with the fourth power of the numerical aperture and cannot be corrected without the use of aspheric optics.

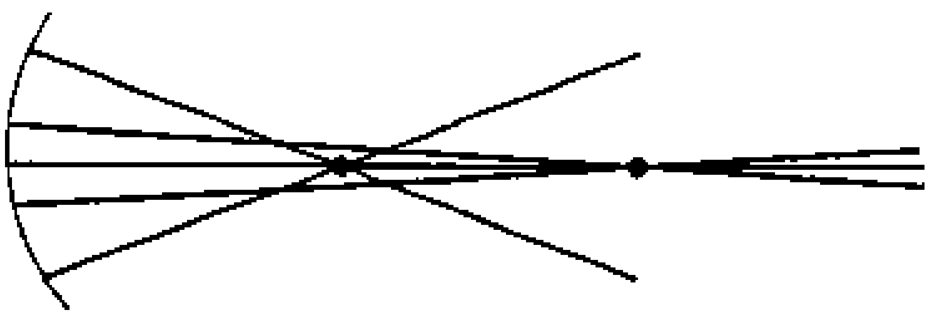


Figure 9 - The Effect of Spherical Aberration

4) Astigmatism is characteristic of an off-axis geometry. In this case a spherical mirror illuminated by a plane wave incident at an angle to the normal (such as mirror M2 in Fig. 7) will present two foci: the tangential focus, F_t, and the sagittal focus, F_S. Astigmatism has the effect of taking a point at the entrance slit and imaging it as a line perpendicular to the dispersion plane at the exit (see Fig. 10), thereby preventing spatial resolution and increasing slit height with subsequent degradation of optical signal-to-noise ratio. The OPD due to astigmatism varies with the square of numerical aperture and the square of the off-axis angle and cannot be corrected without employing aspheric optics.

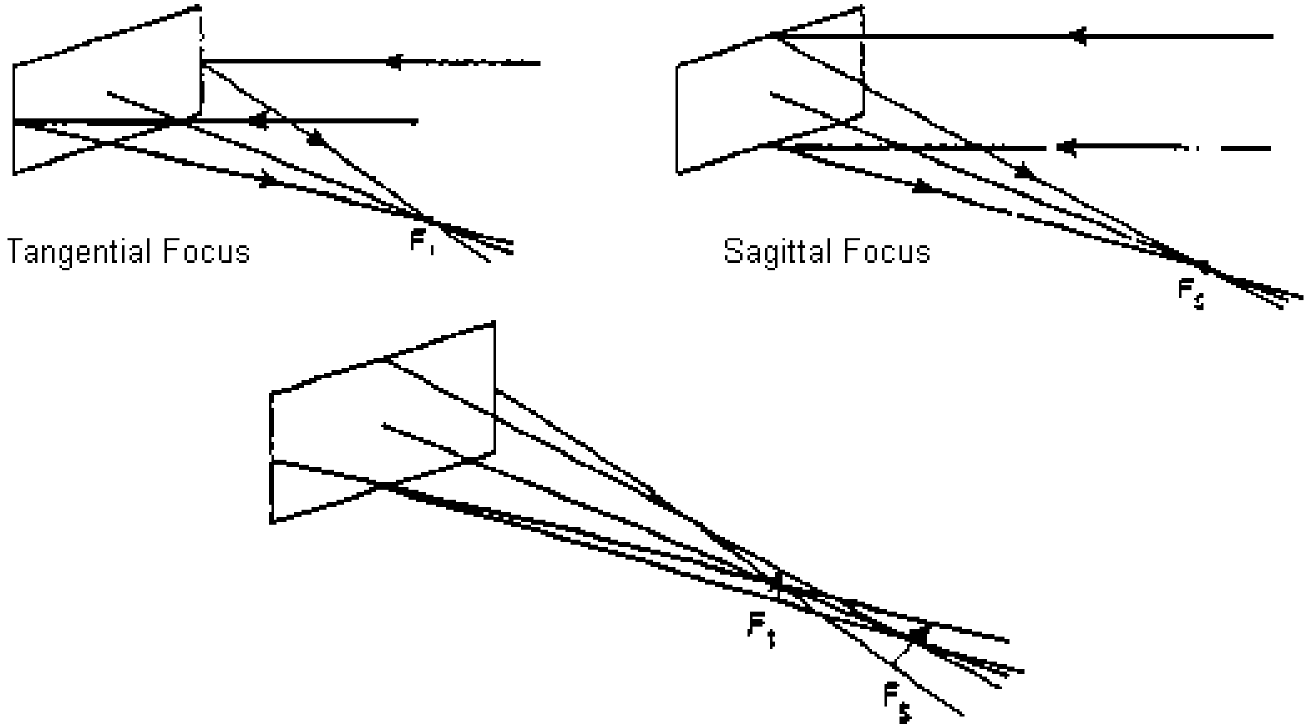


Figure 10 - Effects of Astigmatism in a Concave Mirror Used "Off-Axis"

2.4.1 Aberration Correcting Plane Gratings
Recent advances in holographic grating technology now permits complete correction of ALL aberrations present in a spherical mirror based CZ spectrometer at one wavelength with excellent mitigation over a wide wavelength range (Ref. 12).

2.5 Concave Aberration Corrected Holographic Gratings
Both the monochromators and spectrographs of this type use a single holographic grating with no ancillary optics.

In these systems the grating both focuses and diffracts the incident light.

With only one optic in their design, these devices are inexpensive and compact. Figure 11a illustrates an ACHG monochromator. Figure 11b illustrates an ACHG spectrograph in which the location of the focal plane is established by:

$beta_H$ - Angle between perpendicular to spectral plane and grating normal.

L_H - Perpendicular distance from spectral plane to grating.

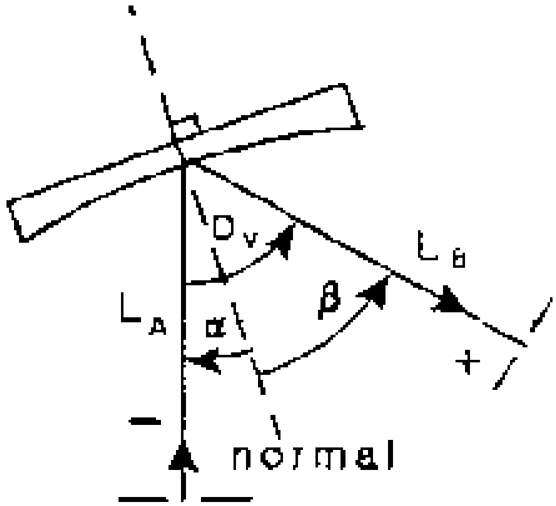


Figure 11a - An ACHG Monochromator

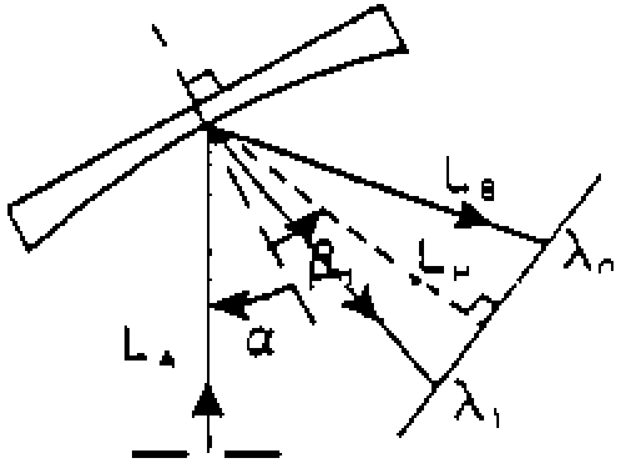


Figure 11b - An ACHG Spectrograph

2.6 Calculating alpha and beta in a Monochromator Configuration

From Equation (1-2),

$$D_V = \beta - \alpha$$

(remains constant)

Taking this equation and Equation (1-3),

$$\alpha = \sin^{-1}\left[\frac{10^{-6}\, kn\lambda}{2\cos(D_V/2)}\right] - \frac{D_V}{2} \quad (2\text{-}1)$$

Use Equations (2-1) and (1-2) to determine alpha and beta, respectively. See Table 3 for worked examples.

Note: In practice the highest wavelength attainable is limited by the mechanical rotation of the grating. This means that doubling the groove density of the grating will halve the spectral range. (See Section 2.14).

2.7 Monochromator System Optics

To understand how a complete monochromator system is characterized, it is necessary to start at the transfer optics that brings light from the source to illuminate the entrance slit. . (See Fig. 12)Here we have "unrolled" the system and drawn it in a linear fashion.

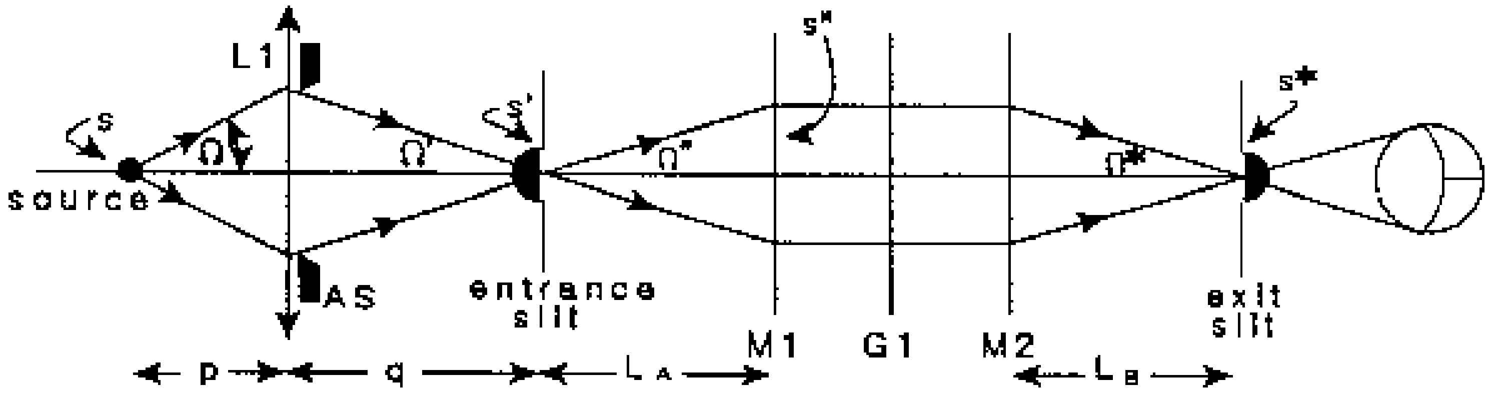


Figure 12 - Typical Monochromator System

AS - aperture stop
L1 - lens 1
M1 - mirror 1
M2 - mirror 2
G1 - grating
p - object distance to lens L1
q - image distance from lens L1
F - focal length of lens L1 (focus of an object at infinity)
d - the clear aperture of the lens (L1 in diagram)
omega - half-angle
s - area of the source
s' - area of the image of the source

2.8 Aperture Stops and Entrance and Exit Pupils

An aperture stop (AS) limits the opening through which a cone of light may pass and is usually located adjacent to an active optic.

A pupil is either an aperture stop or the image of an aperture stop.

The entrance pupil of the entrance (transfer) optics in Fig. 12 is the virtual image of AS as seen axially through lens L1 from the source.

The entrance pupil of the spectrometer is the image of the grating (G1) seen axially through mirror M1 from the entrance slit.

The exit pupil of the entrance optics is AS itself seen axially from the entrance slit of the spectrometer.

The exit pupil of the spectrometer is the image of the grating seen axially through M2 from the exit slit.

2.9 Aperture Ratio (f/value, F.Number), and Numerical Aperture (NA)

The light gathering power of an optic is rigorously characterized by Numerical Aperture(NA).

Numerical Aperture is expressed by:

$$NA = \mu \sin \Omega \tag{2-2}$$

where μ is the refractive index (μ = 1 in air)

and f/value by:

$$f/value = \frac{1}{2NA} \tag{2-3}$$

Table2: Relationship between f/value, half-angle, and numerical aperture

f/value	f/2	f/3	f/5	f/7	f/10	f/15
n (degrees)	14.48	9.6	5.7	4.0	2.9	1.9
NA	0.25	0.16	0.10	0.07	0.05	0.03

2.9.1 f/value of a Lens System
f/value is also given by the ratio of either the image or object distance to the diameter of the pupil. When, for example, a lens is working with finite conjugates such as in Fig. 12, there is an effective f/value from the source to L1 (with diameter AS) given by:

effective f/value$_{in}$= (P/diameter of entrance pupil) = (P/image of AS) (2-4)

and from L1 to the entrance slit by:

effective f/value$_{out}$= (q/diameter of exit pupil) = (q/AS) (2-5)

In the sections that follow f/value will always be calculated assuming that the entrance or exit pupils are equivalent to the aperture stop for the lens or grating and the distances are measured to the center of the lens or grating.

When the f/value is calculated in this way for f/2 or greater (e.g. f/3, f/4, etc.), then sin omega is ~ tan omega and the approximation is good. However, if an active optic is to function at an f/value significantly less than f/2, then the f/value should be determined by first calculating Numerical Aperture from the half-angle.

2.9.2 f/value of a Spectrometer
Because the angle of incidence alpha is always different in either sign or value from the angle of diffraction beta (except in Littrow), the projected size of the grating varies with the wavelength and is different depending on whether it is viewed from the entrance or exit slits. In Figures 13a and 13b, the widths W' and W" are the projections of the grating width as perceived at the entrance and exit slits, respectively.

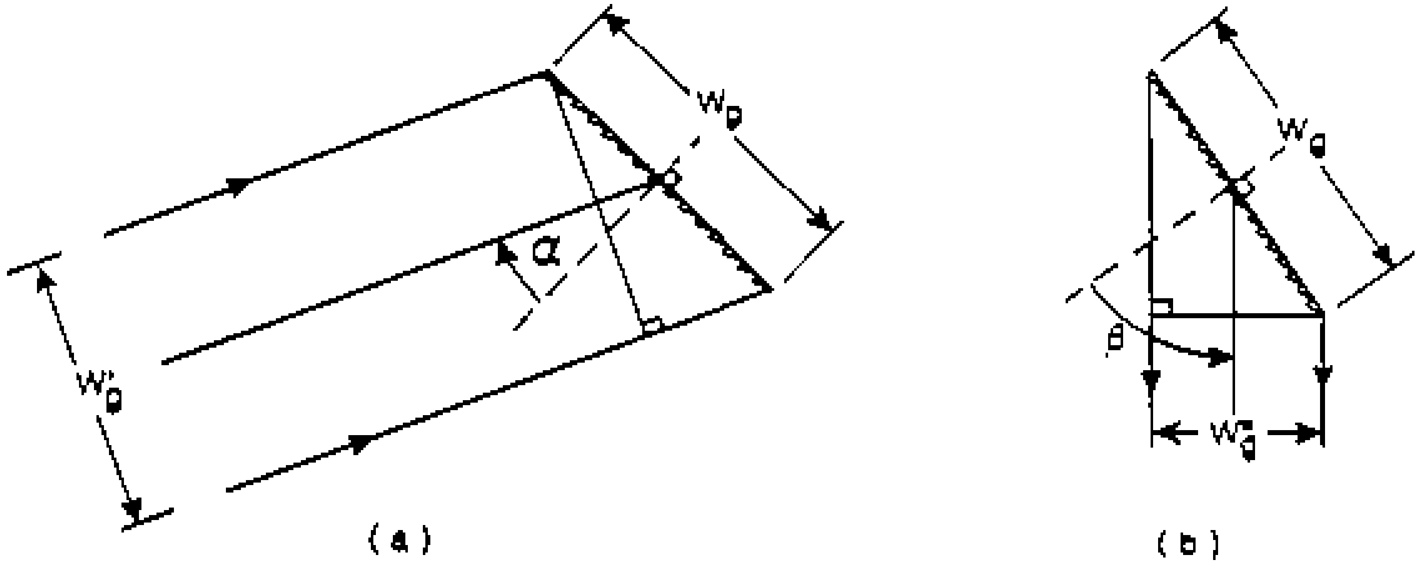


Figure 13 - Projection of the Grating Width on (a) the Entrance and (b) the Exit

To determine the f/value of a spectrometer with a rectangular grating, it is first necessary to calculate the "equivalent diameter", D', as seen from the entrance slit and D" as seen from the exit slit. This is achieved by equating the projected area of the grating to that of a circular disc and then calculating the diameter D' or D".

W'g = Wg cos alpha = projected area of grating from entrance slit (2-6)
W"g = Wg cos beta = projected area of grating from exit slit (2-7)

In a spectrometer, therefore, the $f/value_{in}$ will not equal the $f/value_{out}$.

$f/value_{in} = L_A/D'$(2-8)
$f/value_{out} = L_B/D''$(2-9)

where, for a rectangular grating, D' and D" are given by:

$$D' = 2\sqrt{\frac{W_g H_g \cos\alpha}{\pi}} = 2\sqrt{\frac{W'_g H_g}{\pi}} \quad (2\text{-}10)$$

$$D'' = 2\sqrt{\frac{W_g H_g \cos\beta}{\pi}} = 2\sqrt{\frac{W''_g H_g}{\pi}} \quad (2\text{-}11)$$

where, for a circular grating, D' and D" are given by:

$D' = D_g(\cos alpha)$^(1/2) (2-12)
$D'' = D_g(\cos beta)$^(1/2) (2-13)

Table 3 shows how the f/value changes with wavelength.

Table 3 Calculated values for $f/value_{in}$ and $f/value_{out}$ for a Czerny-Turner configuration with 68 x 68 mm, 1800 g/mm grating and $L_A = L_B = F = 320$ nm. Dv = 24 °.

Lambda(nm)	alpha	beta	$f/value_{in}$	$f/value_{out}$
200	-1.40	22.60	4.17	4.34
320	5.12	29.12	4.18	4.46
500	15.39	39.39	4.25	4.74
680	26.73	50.73	4.41	5.24
800	35.40	59.40	4.62	5.84

2.9.3 Magnification and Flux Density
In any spectrometer system a light source should be imaged onto an entrance slit (aperture) which is then imaged onto the exit slit and so on to the detector, sample, etc. This process inevitably results in the magnification or demagnification of one or more of the images of the light source. Magnification may be determined by the following expansions, taking as an example the source imaged by lens L1 in Fig. 12 onto the entrance slit:

$$\text{magnification} = \sqrt{\frac{S'}{S}} = \frac{f/value_{out}}{f/value_{in}} = \frac{(NA)_{in}}{(NA)_{out}} = \frac{q}{p} \quad (2\text{-}14)$$

Similarly, flux density is determined by the area that the photons in an image occupy, so changes in magnification are important if a flux density sensitive detector or sample are present. Changes in the flux density in an image may be characterized by the ratio of the area of the object, S, to the area of the image, S', from which the following expressions may be derived:

$$\frac{S'}{S} = \left(\frac{q}{p}\right)^2 = \left(\frac{f/value_{out}}{f/value_{in}}\right)^2 = \left(\frac{(NA)_{in}}{(NA)_{out}}\right)^2 \quad (2\text{-}15)$$

These relationships show that the area occupied by an image is determined by the ratio of the square of the f/values. Consequently, it is the EXIT f/value that determines the flux density in the image of an object. Those using photographic film as a detector will recognize these relationships in determining the exposure time necessary to obtain a certain signal-to-noise ratio.

2.10 Exit Slit Width and Anamorphism
Anamorphic optics are those optics that magnify (or demagnify) a source by different factors in the vertical and horizontal planes. (See Fig. 14).

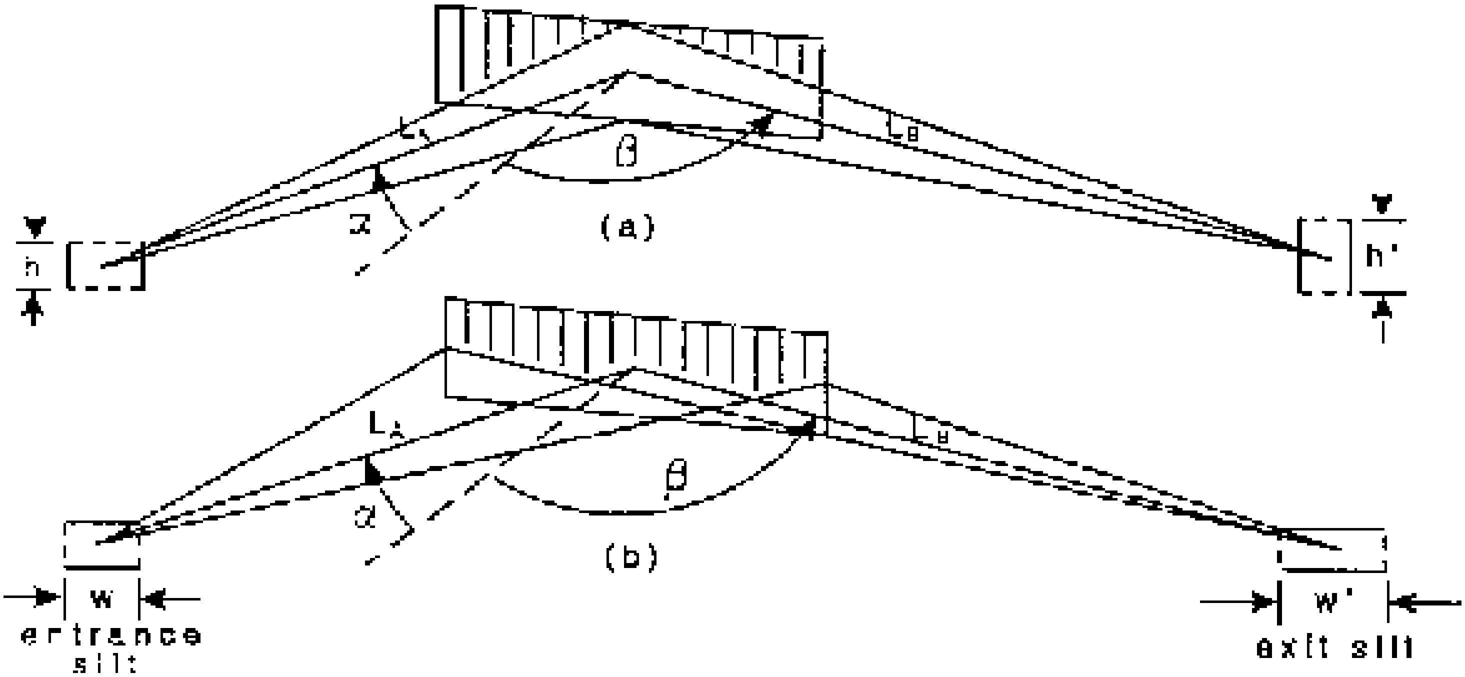


Figure 14 - (a) Vertical and (b) Horizontal Magnification

In the case of a diffraction grating-based instrument, the image of the entrance slit is NOT imaged 1:1 in the exit plane (except in Littrow and perpendicular to the dispersion plane assuming $L_A = L_B$).

This means that in virtually all commercial instruments the tradition of maintaining equal entrance and exit slit widths may not always be appropriate.

Geometric horizontal magnification depends on the ratio of the cosines of the angle of incidence, alpha, and the angle of diffraction, beta, and the L_B/L_A ratio (Equation (2-16)). Magnification may change substantially with wavelength. (See Table 4).

$$w' = w \frac{\cos \alpha}{\cos \beta} \frac{L_B}{L_A} \quad (2\text{-}16)$$

Table 4 illustrates the relationship between alpha, beta, dispersion, horizontal magnification of entrance slit image, and bandpass.

Table 4 Relationship Between Dispersion, Horizontal Magnification, and Bandpass in a Czerny-Turner Monochromator. L_A = 320 mm, L_B = 320 mm, Dv = 24 deg, n = 1800 g/mm Entrance slit width = 1 mm

Wavelength (nm)	alpha (deg.)	beta (deg.)	dispersion (nm/mm)	horiz. magnif.	bandpass* (nm)
200	-1.4	22.60	1.60	1.08	1.74
260	1.84	25.84	1.56	1.11	1.74
320	5.12	29.12	1.46	1.14	1.73
380	8.47	32.47	1.41	1.17	1.72

440	11.88	35.88	1.34	1.21	1.70
500	15.39	39.39	1.27	1.25	1.67
560	19.01	43.01	1.19	1.29	1.64
620	22.78	46.78	1.10	1.35	1.60
680	26.73	50.73	1.00	1.41	1.55
740	30.91	54.91	0.88	1.49	1.49
800	35.40	59.40	1.60	1.60	1.42

Exit slit width matched to image of entrance slit.

*As the inclination of the grating becomes increasingly large, coma in the system will increase. Consequently, in spite of the fact that the bandpass at 800 nm is superior to that at 200 nm, it is unlikely that the full improvement will be seen by the user in systems of less than f/8.

2.11 Slit Height Magnification

Slit height magnification is directly proportional to the ratio of the entrance and exit arm lengths and remains constant with wavelength (exclusive of the effects of aberrations that may be present).

$h' = (L_B/L_A)h$ (2-17)

Note: Geometric magnification is not an aberration!

2.12 Bandpass and Resolution

In the most fundamental sense both bandpass and resolution are used as measure of an instrument's ability to separate adjacent spectral lines.

Assuming a continuum light source, the bandpass (BP) of an instrument is the spectral interval that may be isolated. This depends on many factors including the width of the grating, system aberrations, spatial resolution of the detector, and entrance and exit slit widths.

If a light source emits a spectrum which consists of a single monochromatic wavelength $lambda_o$ (Fig. 15) and is analyzed by a perfect spectrometer, the output should be identical to the spectrum of the emission (Fig. 16) which is a perfect line at precisely $lambda_o$.

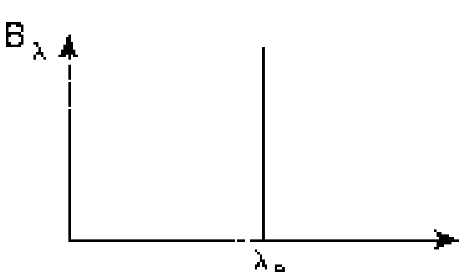


Figure 15 - Real Spectrum of a Monochromatic Light Source

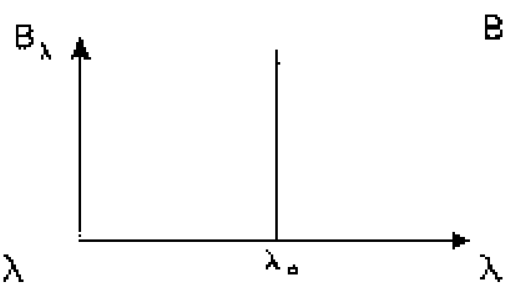
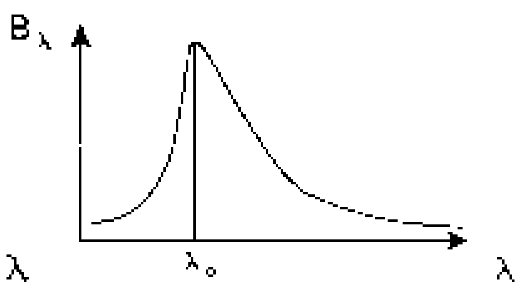


Figure 16 - Recorded Spectrum of a Monochromatic Light Source with a Perfect Instrument



In reality spectrometers are not perfect and produce an apparent spectral broadening of the purely monochromatic wavelength. The line profile now has finite width and is known as the "instrumental line profile" (instrumental bandpass). (See Fig. 17).

The instrumental profile may be determined in a fixed grating spectrograph configuration with the use of a reasonably monochromatic light source such as a single mode dye laser. For a given set of entrance and exit slit parameters, the grating is fixed at the proper orientation for the central wavelength of interest and the laser light source is scanned in wavelength. The output of the detector is recorded and displayed. The resultant trace will show intensity versus wavelength distribution.

For a monochromator the same result would be achieved if a monochromatic light source is introduced into the system and the grating rotated.

The bandpass is then defined as the Full Width at Half Maximum (FWHM) of the trace assuming monochromatic light.

Any spectral structure may be considered to be the sum of an infinity of single monochromatic lines at different wavelengths. Thus, there is a relationship between the instrumental line profile, the real spectrum and the recorded spectrum.

Let B(lambda) be the real spectrum of the source to be analyzed.
Let F(lambda) be the recorded spectrum through the spectrometer.
Let P(lambda) be the instrumental line profile.

F = B * P (2-18)

The recorded function F(lambda) is the convolution of the real spectrum and the instrumental line profile.

The shape of the instrumental line profile is a function of various parameters:

- the width of the entrance slit
- the width of the exit slit or of one pixel in the case of a multichannel detector
- diffraction phenomena
- aberrations
- quality of the system's components and alignment.

Each of these factors may be characterized by a special function Pi(lambda), each obtained by neglecting the other parameters. The overall instrumental line profile P(lambda) is related to the convolution of the individual terms:

P(lambda) = P1(lambda) * P2(lambda) *.....* Pn(lambda) (2-19)

2.12.1 Influence of the Slits (P1(lambda))
If the slits are of finite width and there are no other contributing effects to broaden the line, and if:

W_{ent} = width of the image of the entrance slit
W_{ex} = width of the exit slit or of one pixel in the case of a multichannel detector
delta lambda $_1$ = linear dispersion x W_{ent}
delta lambda $_2$ = linear dispersion x W_{ex}

then the slit's contribution to the instrumental line profile is the convolution of the two slit functions. (See Fig. 18).

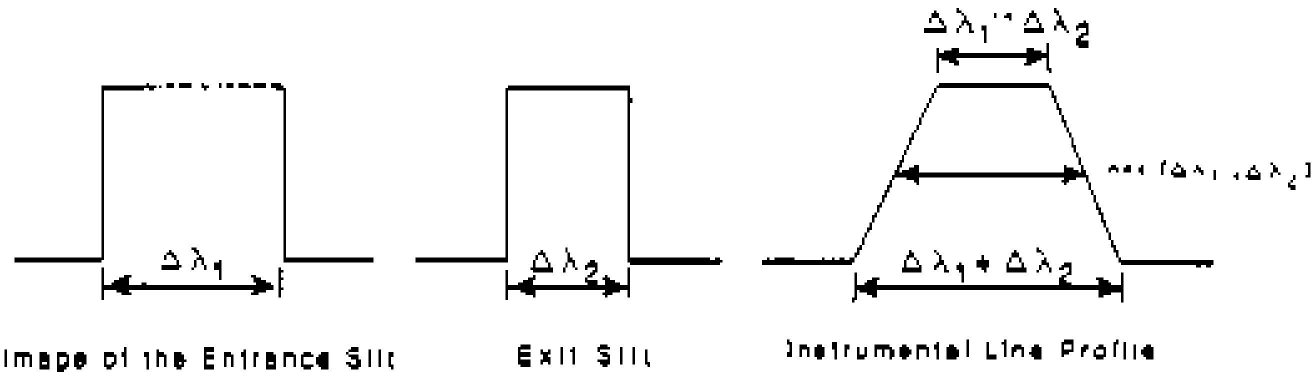


Figure 18 - Convolution of Entrance with Exit Slits

2.12.2 Influence of Diffraction (P2(lambda))

If the two slits are infinitely narrow and aberrations negligible, then the instrumental line profile is that of a classic diffraction pattern. In this case, the resolution of the system is the wavelength, lambda, divided by the theoretical resolving power of the grating, R (Equation 1-11).

2.12.3 Influence of Aberrations (P3(lambda))

If the two slits are infinitely narrow and broadening of the line due to aberrations is large compared to the size due to diffraction, then the instrumental line profile due to diffraction is enlarged.

2.12.4 Determination of the FWHM of the Instrumental Profile

In practice the FWHM of F(lambda) is determined by the convolution of the various causes of line broadening including:

d lambda (resolution): the limiting resolution of the spectrometer is governed by the limiting instrumental line profile and includes system aberrations and diffraction effects.

d lambda (slits): bandpass determined by finite spectrometer slit widths.

d lambda (line): natural line width of the spectral line used to measure the FWHM.

Assuming a gaussian line profile (which is not the case), a reasonable approximation of the FWHM is provided by the relationship:

$$\mathrm{FWHM} \simeq \sqrt{d\lambda^2(\mathrm{slits}) + d\lambda^2(\mathrm{resolution}) + d\lambda^2(\mathrm{line})} \tag{2-20}$$

In general, most spectrometers are not routinely used at the limit of their resolution so the influence of the slits may dominate the line profile. From Fig. 18 the FWHM, due to the slits, is determined by either the image of the entrance slit or the exit slit, whichever is greater. If the two slits are perfectly matched and aberrations minimal compared to the effect of the slits, then the FWHM will be half the width at the base of the peak. (Aberrations may, however, still produce broadening of the base). Bandpass (BP) is then given by:

BP = FWHM ~ linear dispersion x (exit slit width or the image of the entrance slit, whichever is greater).

In Section 2-10 image enlargement through the spectrometer was reviewed. The impact on the determination of the system bandpass may be determined by taking Equation (2-16) to calculate the width of the image of the entrance slit and multiplying it by the dispersion (Equation (1-5)).

Bandpass is then given by:

$$BP = \frac{10^6 \; w \cos \alpha}{kn \; L_A}$$ (2-21)

The major benefit of optimizing the exit slit width is to obtain maximum THROUGHPUT without loss of bandpass.

It is interesting to note from Equations (2-21) and (1-5) that:

- Bandpass varies as cos alpha
- Dispersion varies as cos beta.

2.12.5 Image Width and Array Detectors

Because the image in the exit plane changes in width as a function of wavelength, the user of an array type detector must be aware of the number of pixels per bandpass that are illuminated. It is normal to allocate 3-6 pixels to determine one bandpass. If the image increases in size by a factor of 1.5, then clearly photons contained within that bandpass would have to be collected over 4-9 pixels. For a discussion of the relation between wavelength and pixel position see Section 5. The FWHM that determines bandpass is equivalent to the width of the image of the entrance slit containing a typical maximum of 80% of available photons at the wavelength of interest; the remainder is spread out in the base of the peak. Any image magnification, therefore, equally enlarges the base spreading the entire peak over additional pixels.

2.12.6 Discussion

a) Bandpass with Monochromatic Light

The infinitely narrow natural spectral band width of monochromatic light is, by definition, less than that of the instrumental bandpass determined by Equation (2-20). (A very narrow band width is typically referred to as a "line" because of its appearance in a spectrum).

In this case all the photons present will be at exactly the same wavelength irrespective of how they are spread out in the exit plane. The image of the entrance slit, therefore, will consist exclusively of photons at the same wavelength even though there is a finite FWHM. Consequently, bandpass in this instance cannot be considered as a wavelength spread around the center wavelength. If, for example, monochromatic light at 250 nm is present and the instrumental bandpass is set to produce a FWHM of 5 nm, this does NOT mean 250 nm +/- 2.5 nm because no wavelength other than 250 nm is present. It does mean, however, that a spectrum traced out (wavelength vs. intensity) will produce a "peak" with an apparent FWHM of "5 nm" due to instrumental and NOT spectral line broadening.

b) Bandpass with "Line" Sources of Finite Spectral Width

Emission lines with finite natural spectral bandwidths are routinely found in almost all forms of spectroscopy including emission, Raman, fluorescence, and absorption.

In these cases spectra may be obtained that seem to consist of line emission (or absorption) bands. If, however, one of these "lines" is analyzed with a very high resolution spectrometer, it would be determined that beyond a certain bandpass no further line narrowing would take place indicating that the natural bandwidth had been reached.

Depending on the instrument system the natural bandwidth may or may not be greater than the bandpass determined by Equation (2-20).

If the natural bandwidth is greater than the instrumental bandpass, then the instrument will perform as if the emission "line" is a portion of a continuum. In this case the bandpass may indeed be viewed as a spectral spread of +/- 0.5 BP around a center wavelength at FWHM.

Example 1:
Figure 19 shows a somewhat contrived spectrum where the first two peaks are separated on the recording by 32 mm. The FWHM of the first peak is the same as the second but is less than the third. This implies that the natural bandwidth of the third peak is greater than the bandpass of the spectrometer and would not demonstrate spectral narrowing of its bandwidth even if evaluated with a very high resolution spectrometer.

The first and second peaks, however, may well possess natural bandwidths less than that shown by the spectrometer. In these two cases, the same instrument operating under higher bandpass conditions (narrower slits) may well reveal either additional "lines" that had previously been incorporated into just one band, or a simple narrowing of the bandwidth until either the limit of the spectrometer or the limiting natural bandpass have been reached.

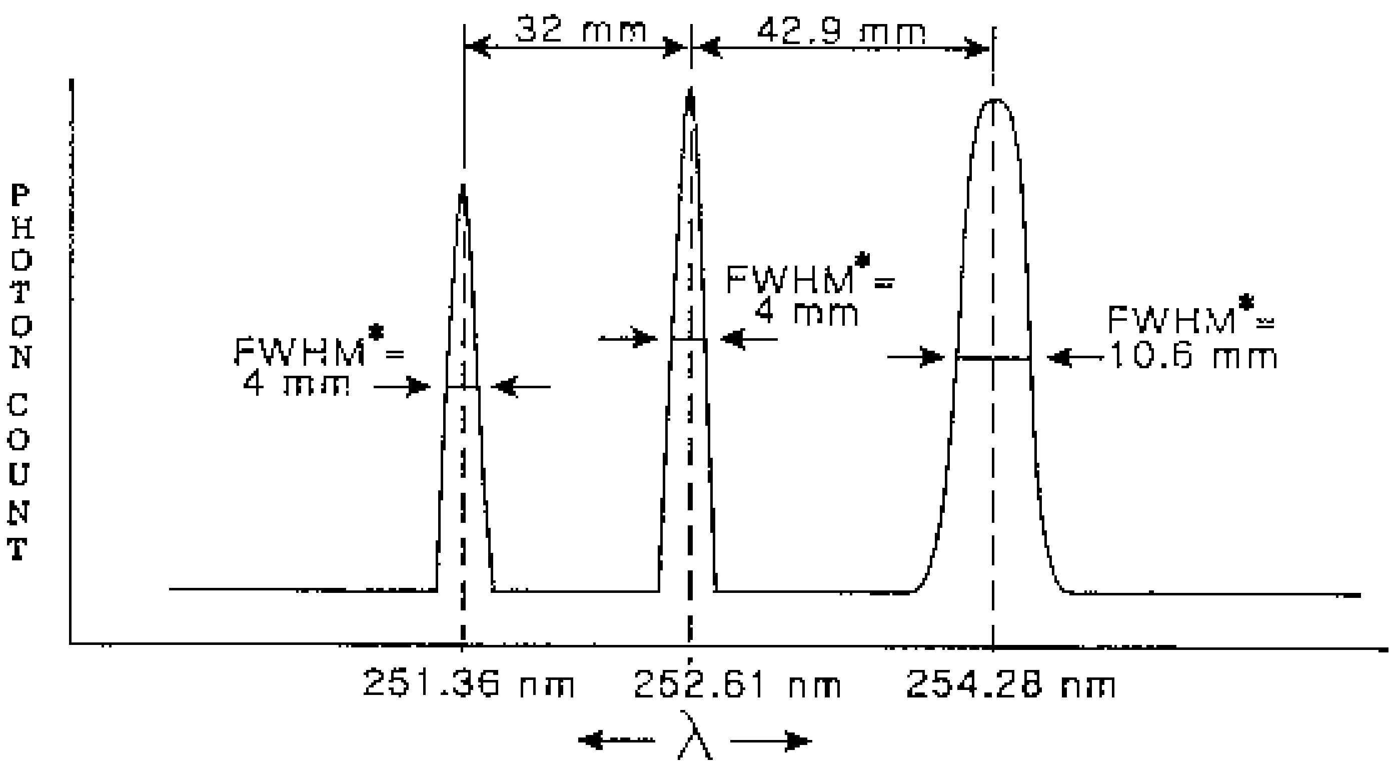


Figure 19 - Strip Chart Recording Plotting Wavelength Versus Intensity where *BP=FWHM (in mm) x Dispersion

Example 2:
A researcher finds a spectrum in a journal that would be appropriate to reproduce on an in-house spectrometer. The first task is to determine the bandpass displayed by the spectrum. If this information is not given, then it is necessary to study the spectrum itself. Assuming that the wavelengths of the two peaks are known, then the distance between them must be measured with a ruler as accurately as possible. If the wavelength difference is found to be 1.25 nm and this increment is spread over 32 mm (see Fig. 19), the recorded dispersion of the spectrum = 1.25/32 = 0.04 nm/mm. It is now possible to determine the bandpass by measuring the distance in mm at the Full Width at Half Maximum height (FWHM). Let us say that this is 4 mm; the bandpass of the instrument is then 4 mm x 0.04 nm/mm = 0.16 nm.

Also assuming that the spectrometer described in Table 4 is to be used, then from Equation (2-21) and the list of maximum wavelengths described in Table 6, the following options are available to produce a bandpass of 0.16 nm:

Table 5: Variation of Dispersion and Slit Width to Produce 0.16 nm Bandpass in a 320 mm Focal Length Czerny-Turner

Groove Density (g/mm)	Dispersion (nm/mm)	Entrance Slit Width (microns)
300	9.2	17
600	4.6	35
1200	2.3	70
1800	1.5	107
2400	1.15	139
3600	0.77	208

The best choice would be the 3600 g/mm option to provide the largest slit width possible to permit the greatest amount of light to enter the system.

2.13 Order and Resolution

If a given wavelength is used in higher orders, for example, from first to second order, it is considered that because the dispersion is doubled, so also is the limiting resolution. In a monochromator in which there are ancillary optics such as plane or concave mirrors, lenses, etc., a linear increase in the limiting resolution may not occur. The reasons for this include:

- Changes in system aberrations as the grating is rotated (e.g., coma)
- Changes in the diffracted wavefront of the grating in higher orders (most serious with classically ruled gratings)
- Residual system aberrations such as spherical aberration, coma, astigmatism, and field curvature swamping grating capabilities (particularly low f/value, e.g., f/3, f/4 systems

Even if the full width at half maximum is maintained, a degradation in line shape will often occur -- the base of the peak usually broadens with consequent degradation of the percentage of available photons in the FWHM.

2.14 Dispersion and Maximum Wavelength

The longest possible wavelength (lambda maxl) an instrument will reach mechanically with a grating of a given groove density is determined by the limit of mechanical rotation of that grating. Consequently, in changing from an original groove density, n_1, to a new groove density, n_2, the new highest wavelength (lambda $_{max2}$) will be:

$$\lambda_{max2} = \lambda_{max1} \frac{n_1}{n_2} \quad (2\text{-}22)$$

Table 6: Variation in Maximum Wavelength with Groove Denisty in a Typical Monochromator

	$L_A = L_B = F = 320$ mm, $D_V = 24$ deg.; In this example maximum wavelength at maximum possible mechanical rotation of a 1200 g/mm grating = 1300 nm	
Groove Density (g/mm)	Dispersion (nm/mm)	Max Wavelength (nm)

150	18.4	10400
300	9.2	5200
600	4.6	2600
1200	2.3	1300
1800	1.5	867
2400	1.15	650
3600	0.77	433

From Table 6 it is clear that if a 3600 g/mm grating is required to diffract light above 433 nm, the system will not permit it. If, however, a dispersion of 0.77 nm/mm is required to produce appropriate resolution at, say, 600 nm, a system should be acquired with 640 mm focal length (Equation (1-5)). This would produce a dispersion of 0.77 nm/mm with a 2400 g/mm grating and also permit mechanical rotation up to 650 nm.

2.15 Order and Dispersion

In Example 2, Section 2.12.6, the solution to the dispersion problem could be solved by using a 2400 g/mm grating in a 640 mm focal length system. As dispersion varies with focal length (L_B), groove density (n), and order (k); for a fixed L_B at a given wavelength, the dispersion equation (Equation 1.5) simplifies to:

kn = constant

Therefore, if first order dispersion = 1.15 nm/mm with a 2400 g/mm grating the same dispersion would be obtained with a 1200 g/mm grating in second order. Keeping in mind that k lambda = constant for a given groove density, n, (Equation 1-9), using second order with an 1800 g/mm grating to solve the last problem would not work because to find 600 nm in second order, it would be necessary to operate at 1200 nm in first order, when it may be seen in Table 6 that the maximum attainable first order wavelength is 867 nm.

However, if a dispersion of 0.77 nm/mm is necessary in the W at 250 nm, this wavelength could be monitored at 500 nm in first order with the 1800 g/mm grating and obtain a second order dispersion of 0.75 nm/mm. In this case any first order light at 500 nm would be superimposed on top of the 250 nm light (and vice-versa). Wavelength selective filters may then be used to eliminate the unwanted radiation.

The main disadvantages of this approach are that the grating efficiency would not be as great as an optimized first order grating and order sorting filters are typically inefficient. If a classically ruled grating is employed, ghosts and stray light will increase as the square of the order.

2.16 Choosing a Monochromator/Spectrograph

Select an instrument based on:

- a) A system that will allow the largest entrance slit width for the bandpass required.
- b) The highest dispersion.
- c) The largest optics affordable.
- d) Longest focal length affordable.
- e) Highest groove density that will accommodate the spectral range.
- f) Optics and coatings appropriate for specific spectral range.
- g) Entrance optics which will optimize etendue.
- h) If the instrument is to be used at a single wavelength in a nonscanning mode, then it must be possible to adjust the exit slit to match the size of the entrance slit image.

Remember: f/value is not always the controlling factor of throughput. For example, light may be collected from a source at f/1 and projected onto the entrance slit of an f/6 monochromator so that the entire image is contained within the slit. Then the system will operate on the basis of the photon collection in the f/l cone and not the f/6 cone of the monochromator. See Section 3.

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Section 3: Spectrometer Throughput and Etendue

3.1 Definitions

Flux - In the spectrometer system flux is given by energy/time (photons/sec, or watts), emitted from a light source or slit of given area, into a solid angle (Q) at a given wavelength (or bandpass).

Intensity (I) - The distribution of flux at a given wavelength (or bandpass) per solid angle (watts/steradian).

Radiance (Luminance) (B) - The intensity when spread over a given surface. Also defined as B = Intensity/Surface Area of the Source (watts/steradian/cm2).

3.1.1 Introduction to Etendue

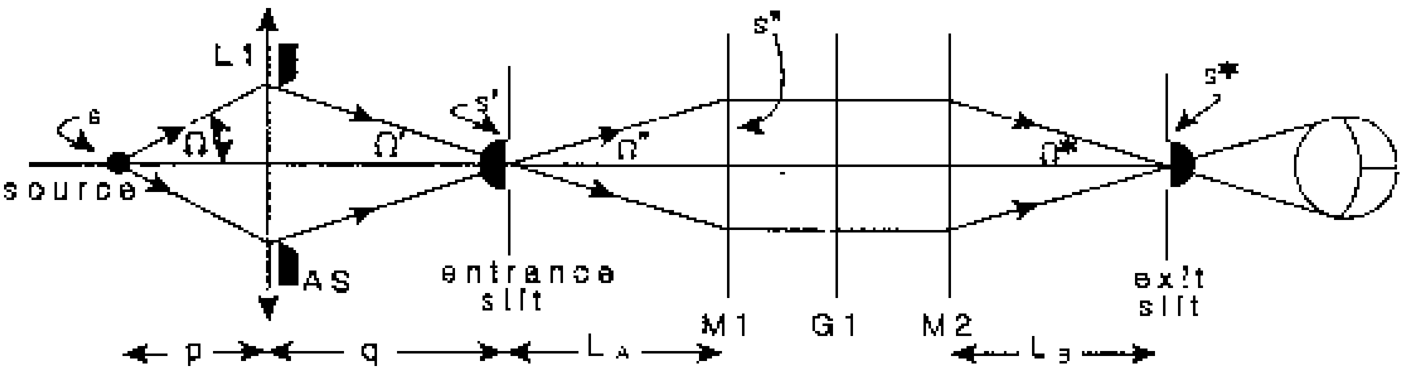

Figure 20 - Typical Monochromator System

S = area of source
S' = area of entrance slit
S '' = area of mirror M1
S* = area of exit slit
omega = half - angle of light collected by L1
omega' = half - angle of light submitted by L1
omega'' = half - angle of light collected by M1
omega* = half - angle of light submitted by M2
L1 = lens used to collect light from source
M1 = spherical collimating Czerny - Turner mirror
M2 = spherical focusing Czerny - Turner mirror
AS = aperture stop
LS = illuminated area of lens L1
p = distance from object to lens L1
q = distance from lens L1 to image of object at the entrance slit
G1 = diffraction grating

Geometric etendue (geometric extent), G, characterizes the ability of an optical system to accept light. It is a function of the area, S, of the emitting source and the solid angle, Q, into which it propagates. Etendue therefore, is a limiting function of system throughput.

$$d^2G = dS\ dQ \quad (3\text{-}1)$$

$$G = \iint dS\ dQ \quad (3\text{-}2)$$

Following integration for a conical beam the axis of which is normal to source of area S (see Fig. 20),

$$G = \pi\ S\ \sin^2\ \Omega \quad (3\text{-}3)$$

Etendue is a constant of the system and is determined by the LEAST optimized segment of the entire optical system. Geometric etendue may be viewed as the maximum beam size the instrument can accept, therefore, it is necessary to start at the light source and ensure that the instrument including ancillary optics collects and propagates the maximum number of photons.

From Equation (3-3), etendue will be optimized if

$$G = \pi\ S\ \sin^2\ \Omega = \pi\ S'\ \sin^2\ \Omega' = \pi\ S''\ \sin^2\ \Omega'' = \pi\ S^*\ \sin^2\ \Omega^* \quad (3\text{-}4)$$

A somewhat simpler approximation may be used if he spectrometer f/value is slower than f/5 (f/6, f/7, etc.).

Then,

$$G \simeq S \times Q \quad (3\text{-}5)$$

where

$$Q = \frac{L_S}{p^2} \quad (3\text{-}6)$$

Then instead of Equation (3-5) we may write

$$G \simeq \frac{S \; L_S}{p^2} - \frac{S' \; L_S}{q^2}$$ etc. (3-7)

This approximation is good when tan omega ~ sin omega ~ (radians). The error at f/5 ~ 1% and at f/1 ~ 33%. Since numerical aperture = u sin omega = NA, then

$$G = \pi \; S \; (NA)^2$$ (3-8)

This form is very useful when working with fiber optics or microscope objectives.

3.2 Relative System Throughput

3.2.1 Calculation of the Etendue

h = height of entrance slit (mm)
w = entrance slit width - bandpass/dispersion (mm)
F = focal length - LA (mm)
n = groove density of grating (g/mm)
G_A = illuminated grating area (mm^2)
S_g = projected illuminated area of grating = G_Ax cos alpha (mm^2)
k = order
BP = bandpass (nm)
S_{ES} = area of entrance slit (mm^2)

The area of entrance slit S_{ES} = w x h (Ref. Equation 2-21) where:

$$w = \frac{k \; n \; F \; BP}{10^6 \; \cos \alpha}$$ (mm) (3-9)

Therefore,

$$S_{ES} = h \frac{k \; n \; F \; BP}{10^6 \; \cos \alpha}$$ (mm2) (3-10)

To calculate etendue, G,

$$G \simeq S_{ES} \; x \; Q$$ (3-11)

and

$$Q = \frac{Sg}{F^2} = \frac{G_A \cos \alpha}{F^2} \quad (3\text{-}12)$$

then

$$G = \frac{h\ n\ k\ G_A\ BP}{F\ 10^6} \quad (3\text{-}13)$$

Relative system throughput is, therefore, proportional to:

- h/F
- groove density (n)
- order (k)
- area of grating (GA)
- bandpass (BP)

The ratio h/F implies that the etendue may be increased by enlarging the height of the entrance slit. In practice this will increase stray light and may also reduce resolution or bandpass resulting from an increase in system aberrations.

3.3 Flux Entering the Spectrometer

Flux is given by radiance times etendue:

$$\Phi = B \times G$$

(3-14, 3-15)

$$\Phi = B\ \pi\ S'\ \sin^2 \Omega'$$

where B is a function of the source, S' is the area of the entrance slit (or emitting source), and omega', is the half cone angle illuminating the spectrometer entrance slit.

Because flux, etendue, and radiance must be conserved between object and image, assuming no other losses, the above terms are all we need to determine the theoretical maximum throughput.

3.4 Example of Complete System Optimization with a Small Diameter Fiber Optic Light Source

First calculate the etendue of the light source:

Given: The fiber has a core diameter of 50 um and emits light with a NA = 0.2 where the area of the fiber core is:

$$S = \pi\ r^2 = \pi\ (0.025)^2 = 1.96 \times 10^{-3}\ mm^2$$

then

$$G = \pi S (NA)^2$$
$$= \pi (1.96 \times 10^{-3}) (0.2)^2$$

Therefore, etendue of the light source = G = 2.46 x 10^{-4}

Next calculate the etendue of the spectrometer assuming a bandpass of 0.5 nm at 500 mm:

n = 1800 g/mm (Given)
k = 1 (Given)
DV = 24° (Given)
LA = F = LB = 320 mm (Given)
GA = 58 x 58 mm ruled area of the grating (Given)
alpha500nm = 15.39° (From Eqn. (2-1))
beta500nn = 39.39° (From Eqn. (1-2))
f/value spectrometer = f/5 (From Eqn. (2-10))
NA spectrometer = 0.1 (From Eqn. (2-3))
f/value fiber optic = f/2.5 (From Eqn. (2-3))
NA fiber optic = 0.2 (Given)
h = to be determined

Calculate operating slit dimensions:

Entrance slit width, w, from Equation (3-9)

$$w = \frac{k\ n\ F\ BP}{10^6 \cos \alpha} = 0.2987 \text{ mm}$$

From (2-16) exit slit width = $w \dfrac{\cos \alpha}{\cos \beta} \times \dfrac{L_B}{L_A}$ = 0.3725

In this case we shall keep the entrance slit height and exit slit height at 0.2987 mm.

The etendue of the spectrometer is given by Equation (3-13).

Then, G = [(0.2987)(1800)(1)(58x58)(0.5)

Consequently, the etendue of the light source (2.46 x 10^{-4}) is significantly less than the etendue of the spectrometer (2.83 x 10^{-3}).

If the fiber was simply inserted between the entrance slit jaws, the NA = 0.2 of the fiber would drastically overfill the NA = 0.1 of the spectrometer (f/2.5 to f/5) both losing photons and creating stray - light. In this case the SYSTEM etendue would be determined by the area of the fiber's core and the NA of the spectrometer.

The point now is to reimage the light emanating from the fiber in such a way that the etendue of the fiber is brought up to that of the spectrometer thereby permitting total capture and propagation of all available photons.

This is achieved with the use of ancillary optics between the fiber optic source and the spectrometer as follows:

$(NA)_{in}$ = NA of Fiber Optic
$(NA)_{out}$ = NA of Spectrometer

then

$$G = \pi S (NA)_{in}^{2} = \pi S' (NA)_{out}^{2}$$

$$\frac{S'}{S} = \left(\frac{q}{p}\right)^2 = \left(\frac{f/value_{out}}{f/value_{in}}\right)^2 = \left(\frac{(NA)_{in}}{(NA)_{out}}\right)^2$$

(2-15)

and $$magnification = \sqrt{\frac{S'}{S}} = \frac{f/value_{out}}{f/value_{in}} = \frac{(NA)_{in}}{(NA)_{out}} = \frac{q}{p}$$

(2-14)
The thin lens equation is

$$\frac{1}{F} = \frac{1}{p} + \frac{1}{q}$$

(3-16)
where F in this case is the focal length for an object at infinity and p and q are finite object and image coordinates. Taking a 60 mm diameter lens as an example where F = 100 mm, then

magnification = NA_{in} / NA_{out} = q / p = 0.2 / 0.2 = 2

Substituting in Equation (3-16)

1 / 100 = 1 / p + 1 /2p

After solving, p = 150 mm and q = 300 mm but

f/$value_{out}$ = 1 / $2(NA)_{out}$ = q / d

then = 300 x 0.2 = 60 mm.

f/$value_{in}$ = 1 / $2(NA)_{in}$ = q / d

then d = 150 x 0.4 = 60 mm.

Therefore, the light from the fiber is collected by a lens with a 150 mm object distance, p, and projects an image of the fiber core on the spectrometer entrance slit 300 mm, q, from the lens. The f/values are matched to both the light propagating from the fiber and to that of the spectrometer. The image, however, is magnified by a factor of 2.

Considering that we require an entrance slit width of 0.2987 mm to produce a bandpass of 0.5 nm, the resulting image of 100 u (2 x 50 u core diam) underfills the slit, thereby ensuring that all the light collected will propagate through the system. As a matter of interest, because the image of the fiber core has a width less than the slit jaws, the bandpass will be determined by the image of the core itself. Stray light will be lessened by reducing the slit jaws to perfectly contain the core's image (see Section 4).

3.5 Example of Complete System Optimization with an Extended Light Source

An "extended light source" is one where the source itself is considerably larger than the slit width necessary to produce an appropriate bandpass. In this case the etendue of the spectrometer will be less than that of the light source.

Using a Hg spectral lamp as an example of an extended source, the etendue 1s as follows:

Area of source = 50 mm (height) x 5 mm (width) (Given)
= 250 mm^2
omega = 90°

Then, $$G = \pi S \sin^2\Omega = \pi\, 250 \sin^2 90° = 785.4$$

Assuming the same spectrometer and bandpass requirements as in the fiber optic source example (3-4) the slit widths and etendue of the spectrometer will also be the same as will the spectrometer etendue. Therefore, the etendue of the light source is drastically larger (785 compared to 2.8 x 10^{-3}) than that of the spectrometer.

Because the etendue of the system is determined by the segment with the LEAST etendue, the maximum light collection from the light source will be governed by the light gathering power of the spectrometer. In the previous example the entrance slit height (h) was taken as 0. 2987 mm. With an extended source, however, it is possible to use a greater slit height, so in this case we will take entrance and exit slit heights of 3 mm. (Even higher slits may be possible but stray light is directly proportional to slit height).

The spectrometer etendue, therefore, increases from 4.7 x 10^{-3} to 4.7 x 10^{-2}

This then will be the effective etendue of the system and will govern the light source. The best way to accommodate this is to sample an area of the of the Hg lamp equivalent to the entrance slit area and image it onto the entrance slit with the same solid angle as that determined by the diffraction grating (Equation (3-12)).

To determine the geometric configuration of the entrance optics take the same 60 mm diameter lens (L1) with a 100 mm focal length as that used in the previous example.

We know that the entrance slit dimensions determine the area of the source to be sampled, therefore, S_{ES} = area of the source S.

The source should be imaged 1:1 onto the entrance slit**,** therefore, magnification = 1.

Taking the thin lens equation

1 / F = 1 / p + 1 / q where q / p = 1

p = 2F and q = 2F

The Hg lamp should be placed 200 mm away from lens L1 which in turn should he 200 mm from the entrance slit.

The diameter required to produce the correct f/value is then determined by the spectrometer whose f/value = 5.

Therefore d = 200 / 5 = 40 mm

The 60 mm lens should, therefore, be aperture stopped down to 40 mm to permit the correct solid angle to enter the spectrometer.

This system will now achieve maximum light collection.

3.6 Variation of Throughput and Bandpass with Slit Widths

Assume: The image of the source overfills the entrance slit.

w_i = original entrance slit width (e.g., 100 um)

w_o = exit slit width (original width of entrance slit image, e.g., 110 um)

3.6.1 Continuous Spectral Source

For example, a tungsten halogen lamp or a spectrum where line widths are significantly greater than instrumental bandpass. (This is often the case in fluorescence experiments.)

Throughput will vary as a function of the product of change in bandpass and change in etendue.

Case 1: Double the entrance slit width, w_i, but keep exit slit unchanged, therefore,

entrance slit = $2w_i$ (200 um)
exit slit = w_o (110 um)

Etendue remains the same (determined by exit slit).
Bandpass is doubled.
Throughput is doubled.

Case 2: Double the exit slit width, w_o, but keep entrance slit unchanged, therefore.

entrance slit = w_i (100 um)

exit slit = $2w_o$ (220 um)

Etendue remains the same (determined by entrance slit).
Bandpass is doubled.
Throughput is doubled.

Note: Doubling the exit slit allows a broader segment of the spectrum through the exit and, therefore, increases the photon flux.

Case 3: Double both the entrance and exit slit widths, therefore,

entrance slit = $2w_i$ (200 um)
exit slit = 2wo (220 um)

Etendue is doubled.
Bandpass is doubled.
Throughput is quadrupled.

3.6.2 Discrete Spectral Source

A light source that will produce a number of monochromatic wavelengths is called a discrete spectral source.

In practice an apparently monochromatic line source is often a discrete segment of a continuum. It is assumed that the natural line width is less than the minimum achievable bandpass of the instrument.

Throughput will then vary as a function of change in etendue and is independent of bandpass.

Case 1: Double the entrance slit width, w_i, but keep exit slit unchanged, therefore,

entrance slit = $2w_i$ (200 um)
exit slit = w_o (110 um)

Etendue remains the same (determined by exit slit)
Bandpass is doubled.
Throughput remains the same.

Case 2: Double the exit slit width, w_o, but keep entrance slit unchanged therefore.

entrance slit = w_i (100 um)
exit slit = w_o (220 um)

Etendue remains the same (determined by entrance slit).
Bandpass is doubled.
Throughput remains the same.

Note: For a discrete spectral source, doubling the exit slit width will not cause a change in the throughput because it does not allow an increase of photon flux for the instrument.

Case 3: Double both the entrance and exit slit widths, therefore,

entrance slit = $2w_i$ (200 um)
exit slit = $2w_o$ (220 um)

Etendue is doubled.

Bandpass is doubled.
Throughput is doubled.

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4 Optical Signal-to-Noise Ratio and Stray Light

Stray light and the effect it has on Optical Signal - to - Noise ratio (S/N) falls into one of two major categories either a) random scatter from mirrors, gratings, etc. or b) directional stray light such as reflections, re - entry spectra, grating ghosts and grating generated focused stray light.

4.1 Random Stray Light

Consider first how much light there is to begin with at the primary wavelength of interest then compare it to other wavelengths that may be present as scatter.

4.1.1 Optical Signal - to - Noise Ratio in a Spectrometer

To determine the ratio of signal - to - noise each of the components must first be quantified.

4.1.2 The Quantification of Signal, phi_u

Flux Entering the Instrument (phi_T):

S_{es} = area of the entrance slit = (hw)
B_T = total radiance of light entering the instrument
G_A = total illuminated area of the grating

Then from Eqns. (3-14), (3-11) and (3-12) total flux entering the instrument is given by:

$$\phi_u = \frac{E_\lambda \, B_\lambda \, G_A \, (h'w') \, \cos\beta \, Tg_\lambda}{L_B^2} \quad (4\text{-}1)$$

So to calculate the flux at a given wavelength that will exit the instrument phi_u, let E_{lambda} be the efficiency of the grating at wavelength lambda and B_{lambda} the radiance of light at wavelength lambda in the focal plane.

Assume now that the area of the exit slit is perfectly matched to the image of the entrance slit.

If S_{ex} = the area of the exit slit = (h'w') (or if a spectrograph, the total area of the pixels).

However, there are many cases when the size of the image of the entrance slit is larger than the exit slit due to image aberrations. Light losses of this kind are "geometric losses" and may be characterized by the transmission through the system Tg.

Tg = 1 for a perfect system.

The flux at a given wavelength collected by the detector is given by:

$$\phi_T = \frac{B_T \, G_A \, (hw) \, \cos\alpha}{L_A^2} \quad (4\text{-}2)$$

where Tg is the geometric transmission at wavelength lambda.

4.1.3 The Quantification of Stray Light, phi_d, and S/N Ratio, phi_u / phi_d

The luminance of randomly scattered light is proportional to the flux per unit area on the scattering optic. To calculate stray light due to random scatter:

Let G = the etendue between the grating and the detector element.

$$G = \frac{G_A\ (h'w')\ \cos\beta}{L_B^2} \quad (4\text{-}3)$$

Let B_d = the radiance of stray light proportional to the total flux density phi_T / G_A

C = a factor which expresses the quality of the optics (including the grating) as a function of random scatter.

$$B_d = \frac{C\ B_T\ (hw)\ \cos\alpha}{L_A^2} \quad (4\text{-}4)$$

Total scattered flux is proportional to the radiance of the scattered light, to the area of the entrance slit, and the solid angle with which the exit slit perceives the illuminated optic.

Random flux is given by : $phi_d = B_d\ G$
then,

$$\phi_d = \frac{C\ B_T\ (hw)\ \cos\alpha\ G_A\ (h'w')\ \cos\beta}{L_A^2\ L_B^2} \quad (4\text{-}5)$$

and the ratio of flux at the wavelength of interest phi_u and the random flux phi_d is:

$$\frac{\phi_u}{\phi_d} = \frac{E_\lambda}{C}\ \frac{B_\lambda}{B_T}\ \frac{L_A^2}{(hw)}\ \frac{Tg_\lambda}{\cos\alpha} \quad (4\text{-}6)$$

4.1.4 Optimization of Signal-to-Noise Ratio

Optimization requires two things: the maximization of (phi_u / phi_d) and the elimination of stray reflections. Taking the terms of Equation (4-6) in turn:

C - Obtain the highest quality optics including a holographic grating if one is available.

E_{lambda} - Ensure that the grating is optimized to be most efficient at the wavelengths of interest.

L_A^2/(hw) - Unfortunately, these may not be totally free parameters because of dispersion and bandpass requirements.

Tg_{lambda} - The dominant cause of image enlargement perpendicular to dispersion is astigmatism. If present, the height of the exit slit must be enlarged to collect all available light with subsequent loss in optical signal - to - noise ratio. New aberration correcting plane gratings for use in certain CZ spectrometers enhance S/N ratio by significantly reducing astigmatism.

B_{lambda}/B_T - This term is the ratio of the brightness at the wavelength of interest lambda to the total brightness of the source. Not usually a user accessible function.

4.1.5 Example of S/N Optimization

This is an exercise in compromise. For example, take a researcher who owns a 500 mm focal length monochromator and is dissatisfied with the signal - to - noise ratio. Equation (4-6) suggests that S/N improvement may be achieved by utilizing a longer focal length instrument; a 1000 mm spectrometer just happens to be available. Assuming the bandpass requirement is constant for both experiments, the groove density, wavelength optimization, and size of the grating is the same, then throughput is halved (from Equation (3-13), all other things being equal, etendue will be proportional to the ratio of the focal lengths).

Optical S/N ratio would be improved by a factor of 2. (From Eqn. (4-6) the ratio of the squares of the focal lengths gives a factor of four and assuming the slit heights remain the same the slit widths in the 1000 mm focal length system would produce double the area of the 500 mm system, thereby, losing a factor of two). The question for the researcher to resolve is whether picking up a factor of 2 in S/N ratio was worth losing half the throughput. In this example, there may also be a reduction in the value of Tg, astigmatism being proportional to the numerical aperture (which in this case would be double that of the 500 mm system).

It is also worth checking the availability of a more sensitive detector. It is sometimes possible to obtain smaller detectors with greater sensitivity than larger ones. If this is the case the total throughput loss may not be as severe as originally anticipated.

4.2 Directional Stray Light

4.2.1 Incorrect Illumination of the Spectrometer

If the optics are overfilled, then a combination of stray reflections off mirror mounts, screw heads, fluorescence from anodized castings, etc. may be expected. The solution is simple: optimize system etendue with well designed entrance optics and use field lenses to conjugate aperture stops (pupils). This is achieved by projecting an image of the aperture stop of the entrance optics via a "field" lens at the entrance slit onto the aperture stop of the spectrometer (usually the grating) and then image the grating onto the aperture stop of the exit optics with a field lens at the exit slit. This is reviewed in Section 6.

4.2.2 Re-entry Spectra

In some CZ monochromator configurations especially with low groove density gratings used in the visible or UV , a diffracted wavelength other than that on which the instrument is set may return to the collimating mirror and be reflected back to the grating where it may be rediffracted and find its way to the exit slit. If this problem is serious, a good solution is to place a mask perpendicular to the grooves across the center of the grating. The mask should be the same height as the slits. If the precise wavelength is known, it is possible to calculate the exact impact point on the grating that the reflected wavelength hits. In this case the only masking necessary is at that point.

A more common example of this problem is found in many spectrometers (irrespective of type) when a linear or matrix array is used as the detector. Reflections back to the grating may be severe. The solution is to either tilt the array up to the point that resolution begins to degrade or if the system is being designed for the first time to work out of plane.

4.2.3 Grating Ghosts

Classically ruled gratings exhibit ghosts and stray light that are focused in the dispersion plane and, therefore, cannot be remedied other than by obtaining a different grating that displays a cleaner performance. One of the best solutions is to employ an ion - etched blazed holographic grating that provides good efficiency at the wavelength of interest and no ghosts whatsoever. What stray light may be present is randomly scattered and not focused.

4.3 S/N Ratio ant Slit Dimensions

This section reviews the effects of slit dimensions on S/N ratio for either a continuum or a monochromatic light source in single or double monochromator. It is assumed that the entrance and exit slit dimensions are matched.

4.3.1 The Case for a SINGLE Monochromator and a CONTINUUM Light Source

*** Variation with Slit Width**

Observation: S/N ratio does NOT vary as a function of slit width.

Explanation: From Eqn. (3-13) and a review of Section 3 signal throughput increases as the square of the slit width. (Slit width determines the entrance etendue and the bandpass. Because, the light source is a continuum the increase in signal varies directly with both bandpass and etendue).

The "noise signal" also varies with the square of the slit widths as shown in Equation (4-5). Consequently, both the signal and the noise change in the same ratio.

*** Variation with Slit Height**

Observation: S/N ratio varies inversely with slit height.

Explanation: Signal throughput varies linearly with slit height (from Equation (3-13)).

Noise, however, varies as the square of slit height (from Equation (4-5)). Consequently, S/N ratio varies inversely with slit height.

4.3.2 The Case for a SINGLE Monochromator and MONOCHROMATIC Light

* **Variation with Slit Width**

Observation: S/N ratio varies inversely with slit width.

Explanation: Signal throughput varies directly with slit width. (Even though bandpass increases, only the etendue governs the number of photons available).

The "noise" is proportional to the square of the slit width. Consequently, S/N ratio is inversely proportional to the slit width.

*** Variation with Slit Height**

Observation: S/N ratio varies inversely with slit height.

Explanation: Signal throughput varies linearly with slit height.

Noise varies as the square of the slit height. Consequently, S/N ratio varies inversely with slit height.

4.3.3 The Case for a DOUBLE Monochromator and a CONTINUUM Light Source

* **Variation with Slit Width**

Observation: S/N ratio varies inversely with slit width.

Explanation: S/N ratio at the exit of the first monochromator does not vary with slit width, however, the light now illuminating the optics of the second monochromator is approximately monochromatic and the S/N ratio will now vary inversely with slit width in the second monochromator.

*** Variation with Slit Height**

Observation: S/N ratio varies as the inverse square of slit height.

Explanation: The S/N ratio varies linearly with slit height at the exit of the first monochromator. The second monochromator viewing "monochromatic" light will also change the S/N ratio inversely with slit height, therefore, the total variation in S/N ratio at the exit of the second monochromator will vary as the square of the slit height.

4.3.4 The Case for a DOUBLE Monochromator and a MONOCHROMATIC Light Source

* **Variation with Slit Width**

Observation: S/N ratio varies with the inverse square of the slit width.

Explanation: At the exit of the first monochromator S/N varies inversely with slit width. The second monochromator also illuminated by monochromatic light again changes the S/N ratio inversely with slit width. Consequently, the total change in S/N ratio is proportional to the inverse square of the slit width.

* **Variation with Slit Height**

Observation: S/N ratio varies with the inverse square of slit height.

Explanation: Each of the two monochromators varies the S/N ratio inversely with slit height so the total variation in S/N ratio varies as the inverse square of the slit height.

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5 The Relationship Between Wavelength and Pixel Position on an Array

For a monochromator system being used in spectrograph configuration with a solid state detector array, the user should be aware of the following

(a) The focal plane may be tilted by an angle, gamma. Therefore, the pixel position normally occupied by the exit slit may NOT mark the normal to the focal plane.

(b) The dispersion and image magnification may vary over the focal plane.

(c) As a consequence of (b), the number of pixels per bandpass may vary not only across the focal plane but will also vary depending on the wavelength coverage.

Figure 21(a) illustrates a tilted focal plane that may be present in Czerny - Turner monochromators. In the case of aberration - corrected holographic gratings, gamma, beta$_H$. and L_H are provided as standard operating parameters.

Operating manuals for many Czerny - Turner (CZ) and Fastie - Ebert (FE) monochromators rarely provide information on the tilt of the focal plane, therefore, it may be necessary for the user to deduce the value of gamma. This is most easily achieved by taking a well - known spectrum and iteratively substituting incremental values of +/- gamma, until the wavelength appearing at each pixel corresponds to calculated values.

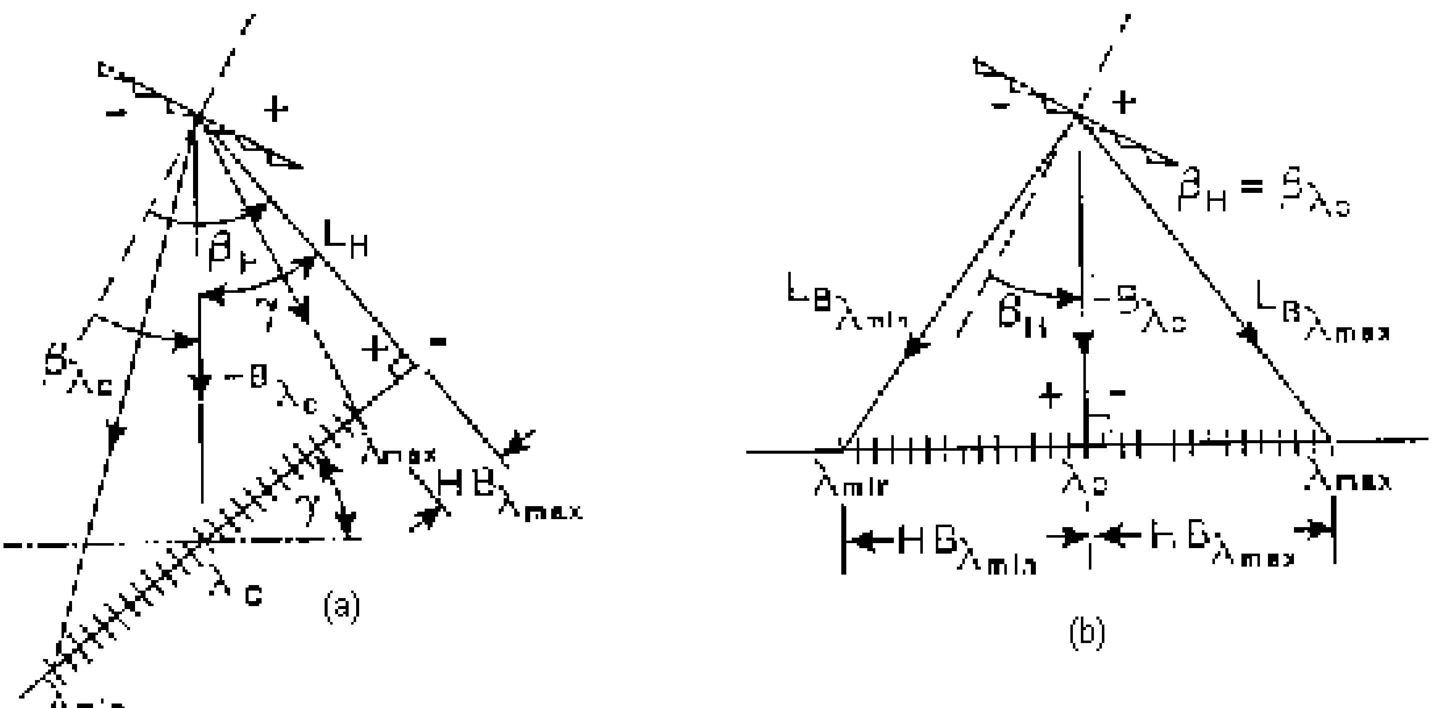

Figure 21 - Spectrograph with Focal Plane (a) inclined and (b) Normal to the Central Wavelength

5.1 The Determination of Wavelength at a Given Location on a Focal Plane

The terms used below are consistent for aberration - corrected holographic concave gratings as well as

Czerny - Turner and Fastie - Ebert spectrometers.

Lambda $_C$ - Wavelength (in nm) at center of array (where exit slit would usually be located)
L_A - Entrance arm length (mm)
$L_{B\ lambda\ n}$ - Exit arm length to each wavelength located on the focal plane (mm)
$L_{B\ lambda\ c}$ - Exit arm length to lambda $_c$ (Czerny - Turner and Fastie - Ebert monochromators $L_A = L_{B\ lambda\ c} = F$)
L_H - Perpendicular distance from grating or focusing mirror to the focal plane (mm)
F - Instrument "focal length". For CZ and FE monochromators $L_A = F = L_B$. (mm)
beta $_H$ - Angle from L_H to the normal to the grating (this will vary in a scanning instrument)
beta $_{lambda\ n}$ - Angle of diffraction at wavelength n
beta $_{lambda\ c}$ - Angle of diffraction at center wavelength
H B $_{lambda\ n}$ - Distance from the intercept of the normal to the focal plane to the wavelength lambda $_n$
H B $_{lambda\ c}$ - Distance from the intercept of the normal to the focal plane to the wavelength lambda $_c$
P_{min} - Pixel # at extremity corresponding to lambda $_{min}$ (e.g., # 1)
P_{max} - Pixel # at extremity corresponding to lambda $_{max}$ (e.g., # 1024)
P_w - Pixel width (mm)
P_c - Pixel # at lambda $_c$ (e.g., # 512)
P_{lambda} - Pixel # at lambda $_n$
Inclination of the focal plane measured at the location normally occupied by the exit slit, lambda $_c$. (This is usually the center of the array. However, provided that the pixel marking this location is known, the array may be placed as the user finds most useful). For this reason, it is very convenient to use a spectrometer that permits simple interchange from scanning to spectrograph by means of a swing - away mirror. The instrument may then be set up with a standard slit using, for example, a mercury lamp. Switching to spectrograph mode enables identification of the pixel, P_c, illuminated by the wavelength previously at the exit slit.

The equations that follow are for Czerny - Turner type instruments where gamma = 0° in one case and gamma does not equal 0 in the other.

Case 1 gamma = 0°.

See Figure 21(b).

$L_H = L_B = F$ at lambda $_c$ (mm)
beta $_H$ = beta at lambda $_c$
HB $_{lambda\ n} = P_w (P_{lambda} - P_c)$ (mm)

HB is negative for wavelengths shorter than lambda $_c$.
HB is positive for wavelengths longer than lambda $_c$.

beta $_{lambda\ n}$ = $beta_H - tan^{-1} (HB_{lambda\ n} / L_H)$ (5-l)

Note: The secret of success (and reason for failure) is frequently the level of understanding of the sign convention. Be consistent, make reasonably accurate sketches whenever possible and be philosophical about the arbitrary nature of the beast.

To make a calculation, alpha and beta at lambda $_c$ can be determined from Equations (1-2) and (2-1). At this point the value for alpha is used in the calculation of all values beta $_{lambda\ n}$ for each wavelength.

Then

$$\frac{\phi_u}{\phi_d} = \frac{E_\lambda}{C} \, \frac{B_\lambda}{B_T} \, \frac{L_A^2}{(hw)} \, \frac{T_{g\lambda}}{\cos\alpha} \quad (5\text{-}2)$$

Case 2: gamma does not equal 0°

See Figure 21(a).

L_H = F cos gamma (where F = L $_{B\ lambda\ c}$) (5-3)
beta$_H$ = beta $_{lambda\ c}$ + gamma (5-4)
HB $_{lambda\ c}$ = F sin gamma (5-5)
HB $_{lambda\ n}$ = P_w (P $_{lambda}$ - P_c) + HB $_{lambda\ c}$ (5-6)
beta $_{lambda\ n}$ = beta$_H$ - tan^{-1} (HB $_{lambda\ n}$ /L_H) (5-7)

Again keeping significant concern for the sign of HB $_{lambda\ n}$, proceed to calculate the value beta $_{lambda\ n}$ after first obtaining alpha at lambda $_c$ Then use Equation (5-2) to calculate lambda $_n$.

IN PRACTICE, THIRD AND FOURTH DECIMAL PLACE ACCURACY IS NECESSARY.

Indeed the longer the instrument's focal length, the greater the contribution of rounding errors.

To illustrate the above discussion a worked example, taken from a readily available commercial instrument, is provided.

Example:

The following are typical results for a focal plane inclined by 2.4° in Czerny - Turner monochromator used in spectrograph mode.

L_B = 320 mm at lambda $_c$ = F
n = 1800 g/mm
D = 24°
L_H = 319.719 mm
gamma = 2.4°
HB $_{lambda\ c}$ = 13.4 mm

Array length = 25.4 mm; lambda $_c$ appears 12.7 mm from end of array
lambda $_{min}$, lambda $_{max}$ = wavelength at array extremities
lambda $_{error\ min,\ max}$ = wavelength thought to be at array extremity if gamma = 0°
Disp = dispersion (Equation (1-5)) (nm/mm)
mag = magnification in dispersion plane (Equation (2-16))

delta lambda (gamma = 0°) lambda $_{min}$ or lambda $_{max}$ - lambda $_{error}$ (nm)
delta d = Actual distance of lambda $_{error}$ from extreme pixel (um)

Table 7 Operating Parameters for a CZ Spectrometer with a 2.4° Tilt at lambda $_c$ on the Spectral Plane Compared to a 0° Tilt.

nm	lambda min 229.9463	lambda c 250	lambda max 269.7469	lambda min 381.4545	lambda c 400	lambda max 418.1236	lambda min 686.1566	lambda c 700	lambda max 713.1999
alpha	**1.29864**			**9.5950**			**28.0963**		
beta H	**27.6986**			**35.9950**			**54.496**		
beta	23.0317	25.2986	27.5732	31.3280	33.5950	35.8695	49.8294	52.0963	54.3707
Disp.	1.59	1.57	1.54	1.48	1.45	1.41	1.12	1.07	1.01
Mag	1.09	1.11	1.13	1.16	1.18	1.22	1.37	1.44	1.51
delta lambda	0.051	0	0.015	0.048	0	0.014	0.037	0	0.011
delta d	+32	0	-10	+32	0	-10	+32	0	-10

5.1.1 Discussion of Results

Examination of the results given in the worked example indicates the following phenomena:

A. If an array with 25 um pixels was used and the focal plane was assumed to be normal to lambda $_c$ rather than the actual 2.4°, at least a one pixel error (32 um) would be present at lambda $_{min}$. (This may not seem like much, but it is incredible how much lost sleep and discussion time has been spent attempting to rationalize this dilemma).

B. A 25 um entrance slit is imaged in the focal plane with a width of 27.25 um (1.09 x 25) at 229.946 nm (when lambda $_c$ = 250 nm) but is imaged with a width of 37.75 um at 713.2 nm (1.51 x 25) (when lambda $_c$ = 700 nm), Indeed in this last case the difference in image width at lambda $_{min}$ compared to lambda $_{max}$ varies by over 10% across the array.

C. If the array did not limit the resolution, then a 25 um entrance slit width would produce a bandpass of 0.04 nm. Given that, in the above example with gamma = 0° rather than 2.4°, the wavelength error at lambda $_{min}$ exceeds 0.04 nm. Therefore, a spectral line at this extreme end of the spectral field could "disappear" the closer lambda $_c$ comes to the location of the exit slit.

D. The spectral coverage over the 25.4 mm array varies in the examples calculated as follows:

lambda $_c$ (nm)	(lambda $_{max}$ - lambda $_{min}$) (nm)
250	39.80
400	36.67
700	27.04

5.1.2 Determination of the Position of a known Wavelength In the Focal Plane

In this case, provided lambda $_c$ is known, alpha, beta$_H$, and L_H may be determined as above. If lambda $_n$ is known, the beta $_{\text{lambda n}}$ may be obtained from the Grating Equation (1-1). Then

HB $_{\text{lambda n}}$ = L_H tan (beta$_H$ - beta $_{\text{lambda n}}$) (5-8)

This formula is most useful for constructing alignment targets with the location of known spectral lines marked on a screen or etched into a ribbon, etc.

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6 Entrance Optics

6.1 Choice of Entrance Optics

While lenses are used in the examples that follow, front surface concave mirrors coated for the spectral region of choice are preferred. A coating such as aluminum is highly reflective from 170 nm to the near IR whereas crown and flint glasses start losing transmission efficiency rapidly below 400 nm. "Achromatic Doublets" are routinely cemented with UV absorbing resins and their anti - reflective coatings often discriminate against the UV below 425 nm. (This is due to the fact that such lenses are often used in cameras where photographic film may be very UV sensitive).

If lenses must be used in the blue to UV , then choose uncoated quartz singlets or air spaced doublets.

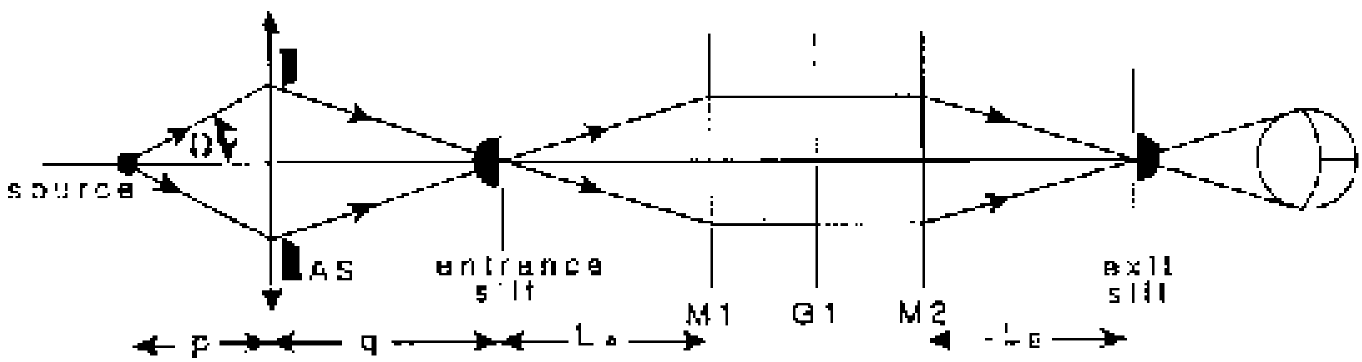


Figure 22 - Typical Monochromator System

AS - aperture stop
L1 - lens 1
M1 - mirror 1
M2 - mirror 2
G1 - grating 1
p - object distance from lens L1
q - image distance from lens L1
F - focal length of lens L1
d - the clear aperture of the lens (L1 in diagram)

The above diagram shows a typical monochromator system with one fixed exit slit and one detector, however, all that follows is equally applicable to a spectrograph.

6.1.1 Review of Basic Equations

Thin lens equation:

$1/F = 1/p + 1/q$ (3-16)

Magnification (m):

$$\text{magnification} = \sqrt{\frac{S'}{S}} = \frac{f/\text{value}_{out}}{f/\text{value}_{in}} = \frac{(NA)_{in}}{(NA)_{out}} = \frac{q}{p} \quad (2\text{-}14)$$

For simplicity the diameter of an optic or that of its aperture stop (AS) (assuming it is very close to the optic itself) is used to determine the f/value. In which case Equations (2-4) and (2-5) simplify to:

$f/value_{in}$ p/d object f/value (6-1)

$f/value_{out}$ q/d image f/value (6-2)

6.2 Establishing the Optical Axis of the Monochromator System

---

6.2.1 Materials

- HeNe laser
- Lenses, mirrors, and other optical components as required for optimization (see Section 3)
- Three pinhole apertures of fixed height above the table
- Precision positioning supports for above
- Optical bench, rail, or jig plate

6.2.2 Procedure

Assemble the above components so that the laser beam acts as the optical axis which passes first through two pinhole apertures, followed by the monochromator, and finally through the third pinhole aperture.

The external optics and source will eventually be placed on the optical axis defined by the pinhole apertures and laser beam. Position the pinhole apertures so that the lenses, etc. may be added without disturbing them.

Note: Reverse illumination may sometimes be preferred where the laser passes first through the exit slit and proceeds through all the optics until it illuminates the light source itself.

Alignment of the components is an iterative process. The goal is for the laser beam to pass through each slit center and to strike the center of each optical element. The following steps achieve this:

1. If a sine drive, then set the monochromator to zero order.
2. Aim the laser beam through the center of the entrance slit.
3. Center the beam on the first optic.
4. Center the beam on the next optic, and so on until it passes through the center of the exit slit.
5. If the laser does not strike the center of the optic following the grating, then rotate the grating until it does. Many spectrometers are not accurately calibrated at zero order, therefore, some offset is to be expected.

6.3 Illuminating a Spectrometer

If a light source such as a sample or a calibration lamp is to be focused into the entrance slit of a spectrometer, then:

* Ensure that the first active optic is homogeneously illuminated. (Plane mirrors are passive).

* Place a white screen between the entrance slit and the first active optic. (In a CZ monochromator the collimating mirror and in an aberration - corrected concave grating the grating itself.) Check for "images", if there is a uniform homogeneously illuminated area, all is well. If not, adjust the entrance optics until there is.

6.4 Entrance Optics Examples

The majority of commercial spectrometers operate between f/3 and f/15, but the diagrams that follow use drawings consistent with f/3 and all the calculations assume f/6.

In the examples which follow, the lens (L1) used is a single thin lens of 100 mm focal length (for an object at infinity) and 60 mm in diameter.

The $f/value_{out}$ of the entrance optics must be equal to the $f/value_{in}$ of the monochromator.

If necessary, an aperture stop should be used to adjust the diameter of the entrance optics.

Remember when calculating the diameter of aperture stops, to slightly underfill the spectrometer optics to prevent stray reflections inside the spectrometer housing.

6.4.1 Aperture Matching a Small Source

Example 1 (Figure 23)

The emitting source is smaller in width than the width of the entrance slit for a required bandpass.

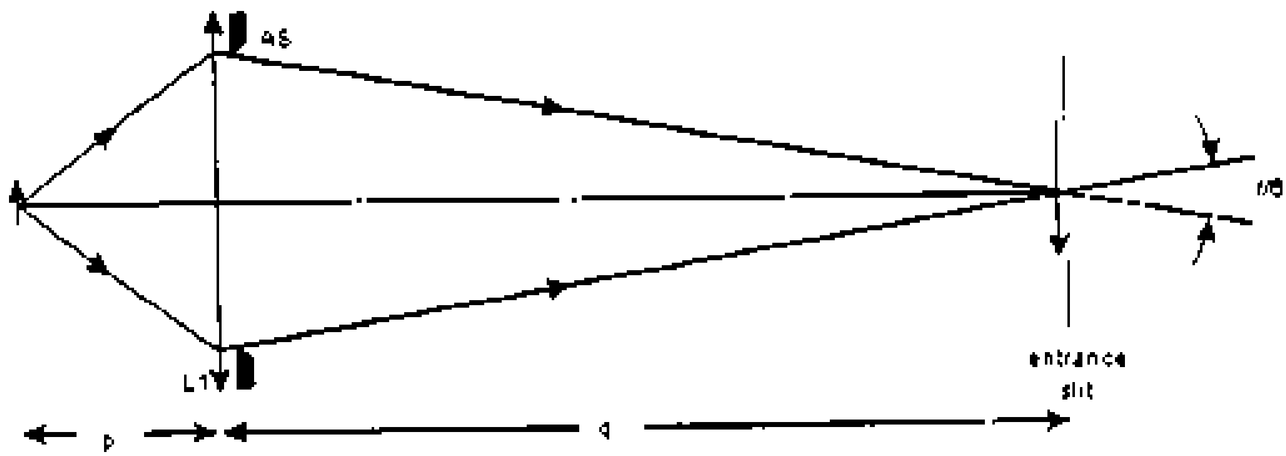


Figure 23 - Small Source Case

1) Calculate the entrance slit-width for appropriate bandpass (Equation (3-9)). For this example, let the slit-width be 0.25 mm.
2) Example Object: a fiber of 0.05 mm core diameter and NA of 0.25.
3) Object emits light at f/2 (NA = 0.25). Spectrometer = f/6.
4) Projected image size of fiber that would be accommodated by the system (given by entrance slit-width) = 0.25 mm.

Calculate magnification to fill entrance slit.
5) m = image size/object size = 0.25/0.05 = 5.O.

Therefore, q/p = 5, q = 5p.

6) Substituting into the lens Equation (3-16) gives p = 120 mm, and q = 600 mm.
7) To calculate d, light must be collected at f/2 and be projected at f/6 to perfectly fill the grating.

Therefore, p/d = 2, d = 120/2 = 60 mm.

Therefore, aperture stop = full diameter of L1.

Projection f/value = 600/60 = 10.

In other words, the grating of the monochromator, even though receiving light collected at f/2, is underfilled by the projected cone at f/10. All the light that could have been collected has been collected and no further improvement is possible.

Example 2

If, however, the fiber emitted light at f/l, light collection could be further improved by using a lens in the same configuration, but 120 mm in diameter. This would, however, produce an output f/value of

600/120 = f/5

Because this exceeds the f/6 of the spectrometer, maximum system light collection would be produced by a lens with diameter

d = q/(f/value) = 600/6 = 100 mm

thereby matching the light collection etendue to the limiting etendue of the spectrometer.

The collection f/value is, therefore,

$f/value_{in}$ = p/q = 120/100 = 1.2

Since etendue is proportional to the square of the $(f/value)^{-l}$, about 70% of the available emitted light would be collected at f/1.2. See Section 3.

If the user had simply placed the fiber at the entrance slit with no entrance optics, only 3': of the available light would have been collected. (Light in this case was collected at the spectrometer's f/6 rather than the f/1.2 with etendue matching entrance optics).

6.4.2 Aperture Matching an Extended Source

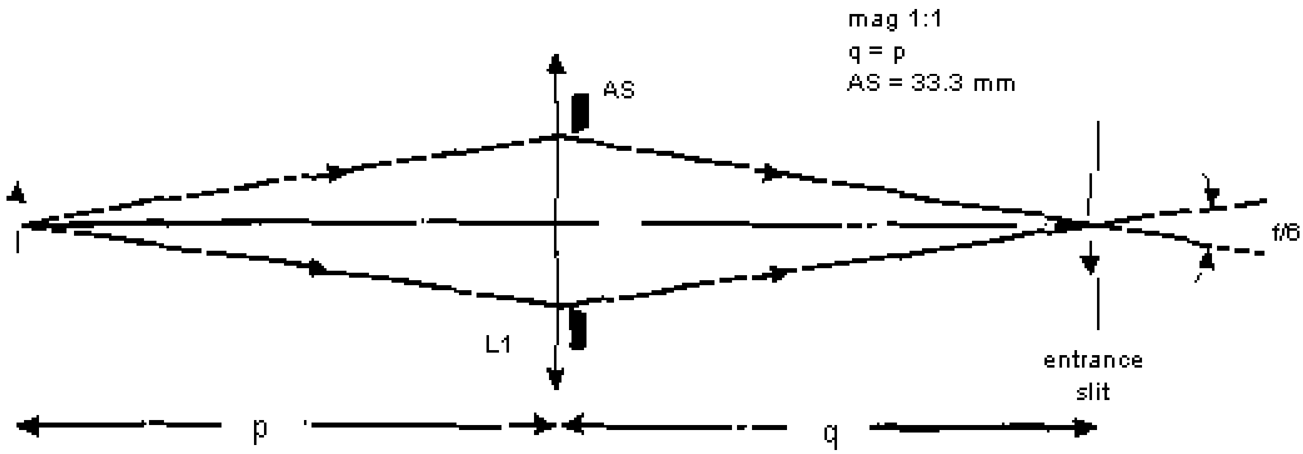


Figure 24 - Extended Source Case

The object width is equal to or greater than the entrance slit width. See Figure 24.

The f/value$_{out}$ of the entrance optics must be equal to the f/value$_{in}$ of the monochromator.

The object distance should be equal to the image distance (absolute magnification, m, equals 1).

Aperture stops should be used to match etendue of the entrance optics to the monochromator .

Because the object is larger than the slit-width, it is the monochromator etendue that will limit light collection.

In this case, image 1:1 at unit magnification.

l) Taking lens L1
So for F = 100 mm, p = 200 mm, q = 200 mm (2F).

2) f/value of the monochromator = q/d = p/d = 6.
3) Then
d f/value = q/(f/value) =200/6 = 33.3

Therefore, aperture stop = 33.33 mm to fill the diffraction grating perfectly.

6.4.3 Demagnifying a Source
In this case the f/value of the source is numerically larger than that of the spectrometer. This is often seen with a telescope which may project at f/30 but is to be monitored by a spectrometer at f/6. In this case etendue matching is achieved by the demagnification of the source. See Figure 25.

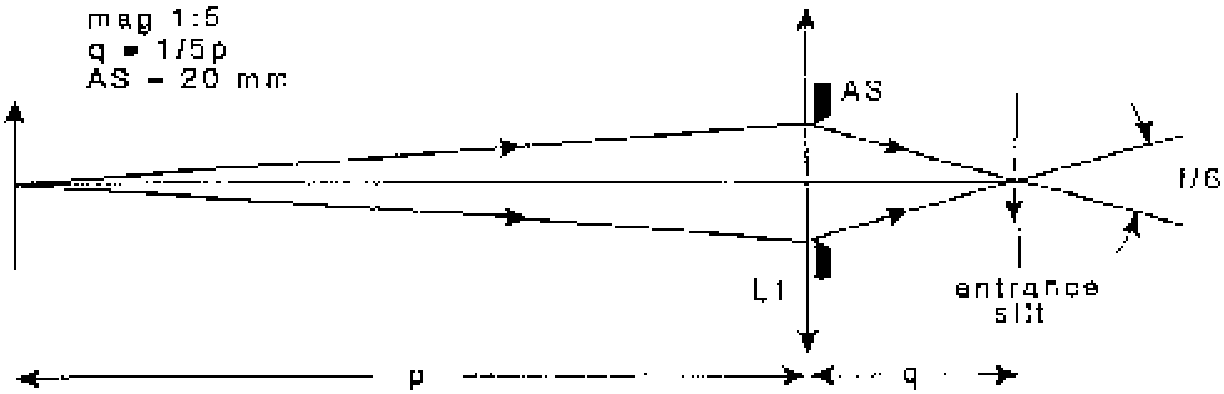


Figure 25 - Demagnified Source Case

1) Calculate the entrance slit-width for the appropriate bandpass(Equation (2-21)). Take, for example, 1.0 mm = final image size = entrance slit width.
2) Image projected by telescope = 5 mm and forms the object for the spectrometer.

m = 1/5 = 0.2,

then from Equation (3-16). Taking lens L1 with F = 100 mm (given),

p = 600 mm, q = 120 mm.

Calculate d knowing the monochromator f/value = 6.

q/d = 6, d = 120/6 = 20 mm.

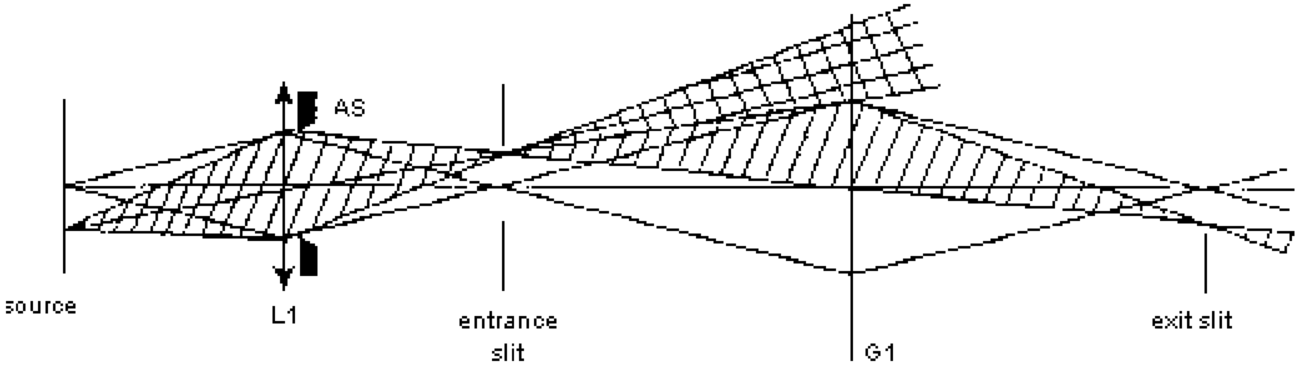
The aperture stop will be 20 mm diameter.

Light is gathered at either the aperture of the projected image or 600/20 = f/30, whichever is numerically greater.

6.5 Use of Field Lenses
The concepts given in this section have not included the use of field lenses. Extended sources often require each pupil in the train to be imaged onto the next pupil downstream to prevent light loss due to overfilling the optics (vignetting). See Section 2.8.

- Used when entrance slit height is large and the light source is extended.
- A field lens images one pupil onto another. In Fig. 26, AS is imaged onto G1.

Field lenses ensure that for an extended source and finite slit height, all light reaches the grating without vignetting. In Figures 26 and 27 the height of the slit is in the plane of the paper.



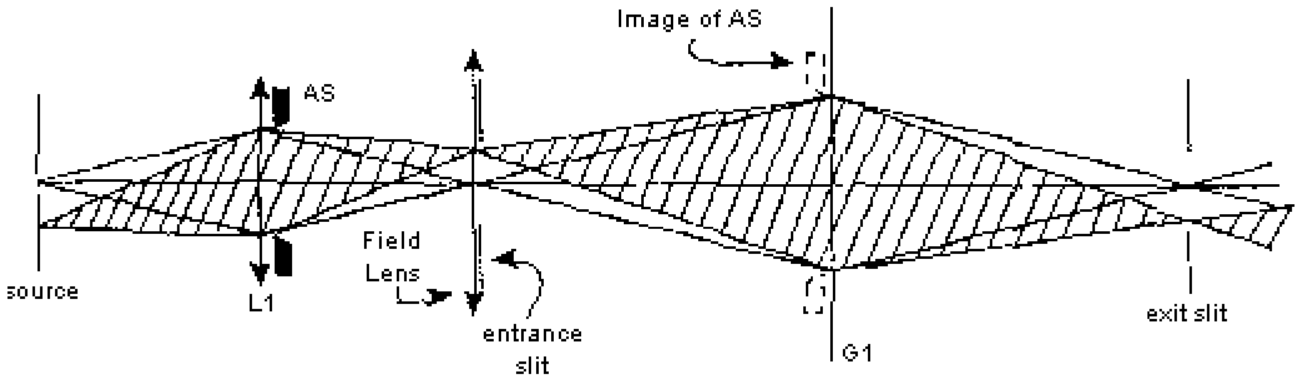


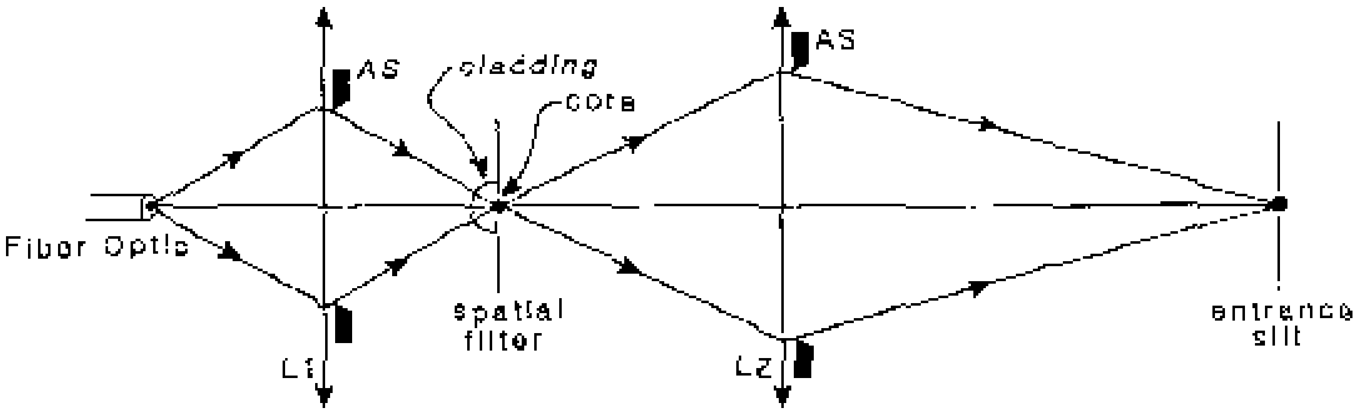
Figure 27 - Example of Illumination System with Field Lens

6.6 Pinhole Camera Effect
When entrance optics are absent, it is possible for the entrance slit to project an image of just about everything before the slit into the spectrometer. This may include the lamp, the sample, rims of lenses, even distant windows. Section 3 describes how to correctly illuminate a spectrometer for highest throughput. Following this procedure will eliminate the pinhole camera effect.

Multiple imaging may severely degrade exit image quality and throughput. On the other hand, the pinhole camera effect is very useful in the VUV when refractive lenses are not available and mirrors would be inefficient.

6.7 Spatial Filters
Aperture and field stops may be used to reduce or even eliminate structure in a light source, and block the unwanted portions of the light (e.g., the cladding around an optical fiber). In this capacity, aperture stops are called spatial filters. See Figure 28.

The light source image is focused onto the plane of the spatial filter. which then becomes the light source for the system.



p = q, (m = 1); p' < q', (m > 1); f/value = q'/d

Figure 28 - Spatial Filter Case

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BIBLIOGRAPHY

l) Diffraction Gratings Ruled and Holograchic Handbook, published by Instruments SA, Inc., 6 Olsen Avenue, Edison, New Jersey 08820 USA and Jobin-Yvon Div. d' Instruments SA., 16-18 Rue du Canal 91160 Longjumeau, France.

2) Chi, Chang H., Ed., "Periodic Structures, Gratings, Moire Patterns and Diffraction Phenomena", SPIE Proc. 240 (1980).

3) Goldstein, S. A. and Walters, J. P., "A Review of Considerations for High Fidelity Imaging of Laboratory Spectroscopic Sources - Parts 1 and 2", Spectrochimica ACTA, 31B, 201-316, (1976).

4) Hecht, E. and A. Zajac, <u>Ontics</u>, Addison Uesley, Reading, Massachusetts, ITRA (19 7 9).

5) James, J. F. and R. S. Sternburg, <u>The Design of Optical Spectrometers</u> Chapman & Hall Ltd., London, England, (1969).

6) Lerner, Jeremy M., Ed., "International Conference on the Application, Theory and Fabrication of Periodic Structures, Diffraction Gratings and Moire Phenomena", SPIE Proc. 503 (1984).

7) Lerner, Jeremy M., Ed., "International Conference on the Application, Theory and Fabrication of Periodic Structures, Diffraction Gratings and Moire Phenomena", SPIE Proc. 815 (1987).

8) Reader, J., "Optimizing Czerny-Turner Spectrographs: A Comparison Between Analytic Theory and Ray Tracing", J. Opt. Soc. Am. 59, (9), 1189-1196. (1969).

9) Reader, J., "What is Dynamic Dispersion", Applied Optics 20, (13), 2173-2172, (1981).

10) Shafer, A. B., Megill, L. R., and Droppleman, L., "Optimization of the Czerny-Turner", J. Opt. Soc. Am. 54, (7), 879-887 (1964).

11) Stroke, G. W., Handbuch der Physik XXIX, Springer Berlin, (1967), (Chapter is in English and is comprehensive).

12) Thevenon, A., Flamand, J., Laude, J. P., Touzet, B., and Lerner, J. M., "Aberration Corrected Plane Gratings", SPIE Proc 815, 136-145, (1987).

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