

2. THE PHYSICS OF DIFFRACTION GRATINGS

Excerpt from Diffraction Grating Handbook -
Copyright 2005 Newport Corporation
Email: gratings.sales@newport.com to receive a complete copy.

2.1. THE GRATING EQUATION

When monochromatic light is incident on a grating surface, it is diffracted into discrete directions. We can picture each grating groove as being a very small, slit-shaped source of diffracted light. The light diffracted by each groove combines to form a set of diffracted wavefronts. The usefulness of a grating depends on the fact that there exists a unique set of discrete angles along which, for a given spacing d between grooves, the diffracted light from each facet is in phase with the light diffracted from any other facet, leading to constructive interference.

Diffraction by a grating can be visualized from the geometry in Figure 2-1, which shows a light ray of wavelength λ incident at an angle α and diffracted by a grating (of groove spacing d , also called the *pitch*) along a set of angles $\{\beta_m\}$. These angles are measured from the grating normal, which is shown as the dashed line perpendicular to the grating surface at its center. The sign convention for these angles depends on whether the light is diffracted on the same side or the opposite side of the grating as the incident light. In diagram (a), which shows a *reflection grating*, the angles $\alpha > 0$ and $\beta_1 > 0$ (since they are measured counter-clockwise from the grating normal) while the angles $\beta_0 < 0$ and $\beta_{-1} < 0$ (since they are measured clockwise from the grating normal). Diagram (b) shows the case for a *transmission grating*.

By convention, angles of incidence and diffraction are measured *from* the grating normal *to* the beam. This is shown by arrows in the diagrams. In both diagrams, the sign convention for angles is shown by the plus and minus symbols located on either side of the grating normal. For either reflection or transmission gratings, the algebraic signs of two angles differ if they are measured from opposite sides of the grating normal. Other sign conventions exist, so care must be taken in calculations to ensure that results are self-consistent.

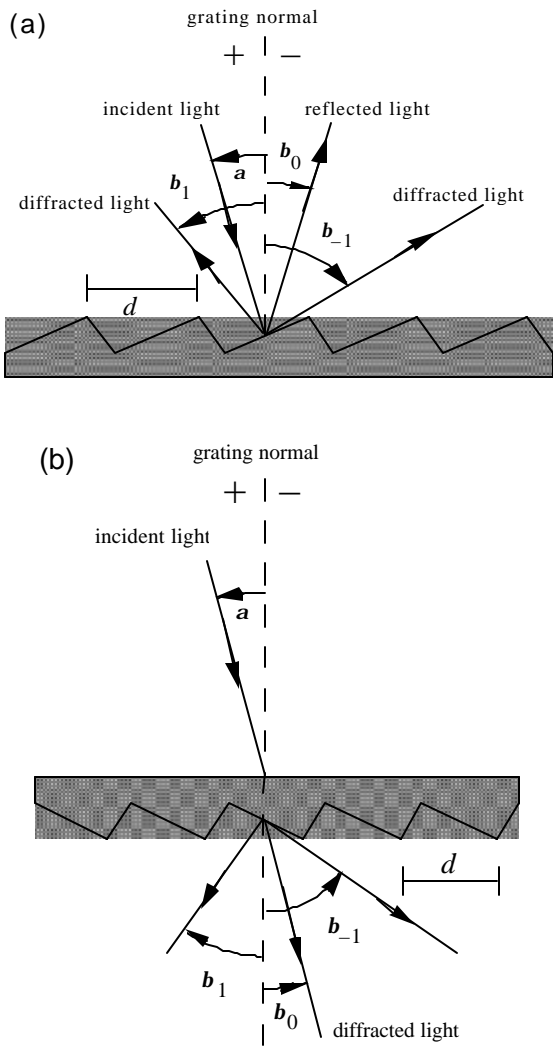


Figure 2-1. Diffraction by a plane grating. A beam of monochromatic light of wavelength λ is incident on a grating and diffracted along several discrete paths. The triangular grooves come out of the page; the rays lie in the plane of the page. The sign convention for the angles a and b is shown by the + and - signs on either side of the grating normal. (a) A reflection grating: the incident and diffracted rays lie on the same side of the grating. (b) A transmission grating: the diffracted rays lie on the opposite side of the grating from the incident ray.

Another illustration of grating diffraction, using wavefronts (surfaces of constant phase), is shown in Figure 22. The geometrical path difference

between light from adjacent grooves is seen to be $d \sin a + d \sin b$. [Since $b < 0$, the term $d \sin b$ is negative.] The principle of constructive interference dictates that only when this difference equals the wavelength λ of the light, or some integral multiple thereof, will the light from adjacent grooves be in phase (leading to constructive interference). At all other angles the wavelets originating from the groove facets will interfere destructively.

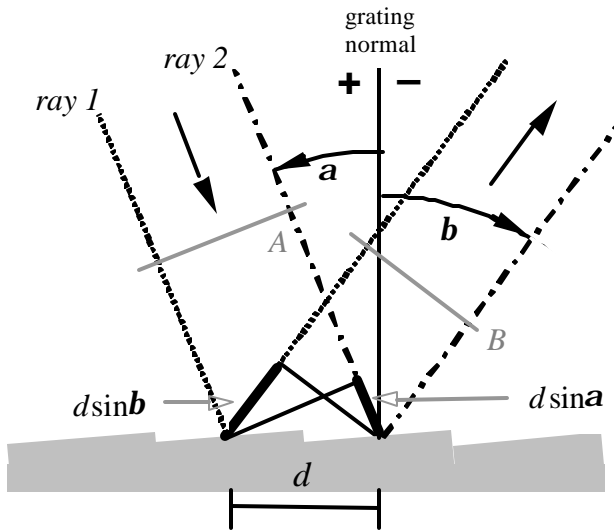


Figure 2-2. Geometry of diffraction, for planar wavefronts. Two parallel rays, labeled 1 and 2, are incident on the grating one groove spacing d apart and are in phase with each other at wavefront A. Upon diffraction, the principle of constructive interference implies that these rays are in phase at diffracted wavefront B if the difference in their path lengths, $dsina + dsinb$, is an integral number of wavelengths; this in turn leads to the grating equation.

These relationships are expressed by the *grating equation*

$$m\lambda = d (\sin a + \sin b), \quad (2-1)$$

which governs the angular locations of the principal intensity maxima when light of wavelength λ is diffracted from a grating of groove spacing d . Here m is the *diffraction order* (or *spectral order*), which is an integer. For a particular

wavelength λ , all values of m for which $|m\lambda/d| < 2$ correspond to propagating (rather than evanescent) diffraction orders. The special case $m = 0$ leads to the law of reflection $\mathbf{b} = -\mathbf{a}$.

It is sometimes convenient to write the grating equation as

$$G\lambda = \sin \mathbf{a} + \sin \mathbf{b}, \quad (2-2)$$

where $G = 1/d$ is the *groove frequency* or *groove density*, more commonly called "grooves per millimeter".

Eq. (2-1) and its equivalent Eq. (2-2) are the common forms of the grating equation, but their validity is restricted to cases in which the incident and diffracted rays lie in a plane which is perpendicular to the grooves (at the center of the grating). The majority of grating systems fall within this category, which is called *classical* (or *in-plane*) *diffraction*. If the incident light beam is not perpendicular to the grooves, though, the grating equation must be modified:

$$G\lambda = \cos \epsilon (\sin \mathbf{a} + \sin \mathbf{b}). \quad (2-3)$$

Here ϵ is the angle between the incident light path and the plane perpendicular to the grooves at the grating center (the plane of the page in Figure 2-2). If the incident light lies in this plane, $\epsilon = 0$ and Eq. (2-3) reduces to the more familiar Eq. (2-2). In geometries for which $\epsilon \neq 0$, the diffracted spectra lie on a cone rather than in a plane, so such cases are termed *conical diffraction*.

For a grating of groove spacing d , there is a purely mathematical relationship between the wavelength and the angles of incidence and diffraction. In a given spectral order m , the different wavelengths of polychromatic wavefronts incident at angle \mathbf{a} are separated in angle:

$$\mathbf{b}(\lambda) = \sin^{-1} \left(\frac{m\lambda}{d} - \sin \mathbf{a} \right). \quad (2-4)$$

When $m = 0$, the grating acts as a mirror, and the wavelengths are not separated ($\mathbf{b} = -\mathbf{a}$ for all λ); this is called *specular reflection* or simply the *zero order*.

A special but common case is that in which the light is diffracted back toward the direction from which it came (i.e., $\mathbf{a} = \mathbf{b}$); this is called the *Littrow configuration*, for which the grating equation becomes

$$m\lambda = 2d \sin \alpha, \quad \text{in Littrow.} \quad (2-5)$$

In many applications a constant-deviation monochromator mount is used, in which the wavelength λ is changed by rotating the grating about the axis coincident with its central ruling, with the directions of incident and diffracted light remaining unchanged. The *deviation angle* $2K$ between the incidence and diffraction directions (also called the *angular deviation*) is

$$2K = \alpha - \beta = \text{constant}, \quad (2-6)$$

while the *scan angle* ϕ which varies with λ and is measured from the grating normal to the bisector of the beams, is

$$2\phi = \alpha + \beta. \quad (2-7)$$

Note that ϕ changes with λ (as do α and β). In this case, the grating equation can be expressed in terms of ϕ and the *half deviation angle* K as

$$m\lambda = 2d \cos K \sin \phi \quad (2-8)$$

This version of the grating equation is useful for monochromator mounts (see Chapter 7). Eq. (2-8) shows that the wavelength diffracted by a grating in a monochromator mount is directly proportional to the sine of the scan angle ϕ through which the grating rotates, which is the basis for monochromator drives in which a *sine bar* rotates the grating to scan wavelengths (see Figure 2-3).

For the constant-deviation monochromator mount, the incidence and diffraction angles can be expressed simply in terms of the scan angle ϕ and the half-deviation angle K via

$$\alpha(\lambda) = \phi(\lambda) + K \quad (2-9)$$

and

$$\beta(\lambda) = \phi(\lambda) - K, \quad (2-10)$$

where we show explicitly that α , β and ϕ depend on the wavelength λ .

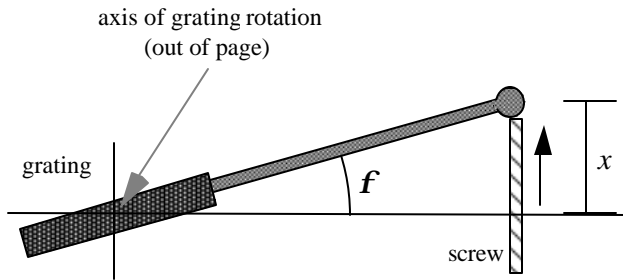


Figure 2-3. A sine bar mechanism for wavelength scanning. As the screw is extended linearly by the distance x shown, the grating rotates through an angle f in such a way that $\sin f$ is proportional to x .

2.2. DIFFRACTION ORDERS

Generally several integers m will satisfy the grating equation – we call each of these values a *diffraction order*.

2.2.1. Existence of diffraction orders

For a particular groove spacing d , wavelength λ and incidence angle α , the grating equation (2-1) is generally satisfied by more than one diffraction angle β . In fact, subject to restrictions discussed below, there will be several discrete angles at which the condition for constructive interference is satisfied. The physical significance of this is that the constructive reinforcement of wavelets diffracted by successive grooves merely requires that each ray be retarded (or advanced) in phase with every other; this phase difference must therefore correspond to a real distance (path difference) which equals an integral multiple of the wavelength. This happens, for example, when the path difference is one wavelength, in which case we speak of the positive first diffraction order ($m = 1$) or the negative first diffraction order ($m = -1$), depending on whether the rays are advanced or retarded as we move from groove to groove. Similarly, the second order ($m = 2$) and negative second order ($m = -2$) are those for which the path

difference between rays diffracted from adjacent grooves equals two wavelengths.

The grating equation reveals that only those spectral orders for which $|m\lambda/d| < 2$ can exist; otherwise, $|\sin \mathbf{a} + \sin \mathbf{b}| > 2$, which is physically meaningless. This restriction prevents light of wavelength λ from being diffracted in more than a finite number of orders. Specular reflection ($m = 0$) is always possible; that is, the *zero order* always exists (it simply requires $\mathbf{b} = -\mathbf{a}$). In most cases, the grating equation allows light of wavelength λ to be diffracted into both negative and positive orders as well. Explicitly, spectra of all orders m exist for which

$$-2d < m\lambda < 2d, \quad m \text{ an integer.} \quad (2-11)$$

For $\lambda/d \ll 1$, a large number of diffracted orders will exist.

As seen from Eq. (2-1), the distinction between negative and positive spectral orders is that

$$\begin{aligned} \mathbf{b} > -\mathbf{a} & \quad \text{for positive orders } (m > 0), \\ \mathbf{b} < -\mathbf{a} & \quad \text{for negative orders } (m < 0), \\ \mathbf{b} = -\mathbf{a} & \quad \text{for specular reflection } (m = 0). \end{aligned} \quad (2-12)$$

This sign convention for m requires that $m > 0$ if the diffracted ray lies to the left (the counter-clockwise side) of the zero order ($m = 0$), and $m < 0$ if the diffracted ray lies to the right (the clockwise side) of the zero order. This convention is shown graphically in Figure 2-4.

2.2.2. Overlapping of diffracted spectra

The most troublesome aspect of multiple order behavior is that successive spectra overlap, as shown in Figure 2-5. It is evident from the grating equation

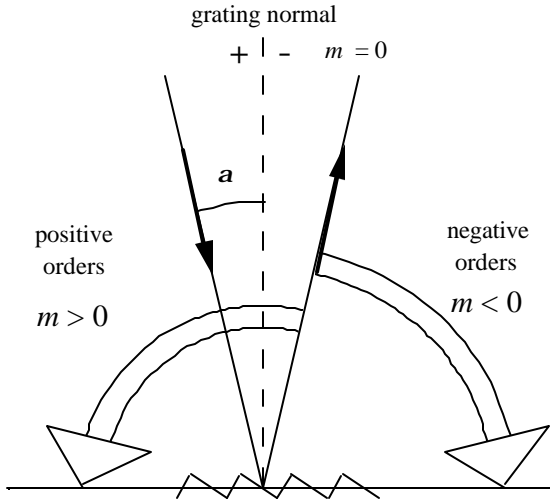


Figure 2-4. Sign convention for the spectral order m . In this example a is positive.

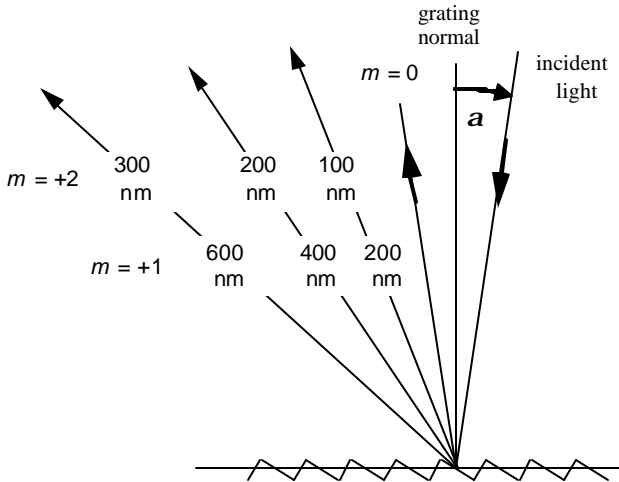


Figure 2-5. Overlapping of spectral orders. The light for wavelengths 100, 200 and 300 nm in the second order is diffracted in the same direction as the light for wavelengths 200, 400 and 600 nm in the first order. In this diagram, the light is incident from the right, so $a < 0$.

that light of wavelength λ diffracted by a grating along direction θ will be accompanied by integral fractions $\lambda/2$, $\lambda/3$, etc.; that is, for any grating instrument configuration, the light of wavelength λ diffracted in the $m = 1$ order will coincide with the light of wavelength $\lambda/2$ diffracted in the $m = 2$ order, etc. In this example, the red light (600 nm) in the first spectral order will overlap the ultraviolet light (300 nm) in the second order. A detector sensitive at both wavelengths would see both simultaneously. This superposition of wavelengths, which would lead to ambiguous spectroscopic data, is inherent in the grating equation itself and must be prevented by suitable filtering (called *order sorting*), since the detector cannot generally distinguish between light of different wavelengths incident on it (within its range of sensitivity). [See also Section 2.7 below.]

2.3. DISPERSION

The primary purpose of a diffraction grating is to disperse light spatially by wavelength. A beam of white light incident on a grating will be separated into its component wavelengths upon diffraction from the grating, with each wavelength diffracted along a different direction. *Dispersion* is a measure of the separation (either angular or spatial) between diffracted light of different wavelengths. Angular dispersion expresses the spectral range per unit angle, and linear resolution expresses the spectral range per unit length.

2.3.1. Angular dispersion

The angular spread $\Delta\theta$ of a spectrum of order m between the wavelength λ and $\lambda + \Delta\lambda$ can be obtained by differentiating the grating equation, assuming the incidence angle α to be constant. The change D in diffraction angle per unit wavelength is therefore

$$D = \frac{d\theta}{d\lambda} = \frac{m}{d \cos\theta} = \frac{m}{d} \sec\theta = Gm \sec\theta, \quad (2-13)$$

where θ is given by Eq. (2-4). The quantity D is called the *angular dispersion*. As the groove frequency $G = 1/d$ increases, the angular dispersion increases (meaning that the angular separation between wavelengths increases for a given order m).

In Eq. (2-13), it is important to realize that the quantity m/d is not a ratio which may be chosen independently of other parameters; substitution of the grating equation into Eq. (2-13) yields the following general equation for the angular dispersion:

$$D = \frac{db}{dI} = \frac{\sin \mathbf{a} + \sin \mathbf{b}}{I \cos \mathbf{b}}. \quad (2-14)$$

For a given wavelength, this shows that the angular dispersion may be considered to be solely a function of the angles of incidence and diffraction. This becomes even more clear when we consider the Littrow configuration ($\mathbf{a} = \mathbf{b}$), in which case Eq. (2-14) reduces to

$$D = \frac{db}{dI} = \frac{2}{I} \tan \mathbf{b}, \quad \text{in Littrow.} \quad (2-15)$$

When $|\mathbf{b}|$ increases from 10° to 63° in Littrow use, the angular dispersion can be seen from Eq. (2-15) to increase by a factor of ten, regardless of the spectral order or wavelength under consideration. Once the diffraction angle \mathbf{b} has been determined, the choice must be made whether a fine-pitch grating (small d) should be used in a low diffraction order, or a coarse-pitch grating (large d) such as an echelle grating (see Section 12.5) should be used in a high order. [The fine-pitched grating, though, will provide a larger free spectral range; see Section 2.7 below.]

2.3.2. Linear dispersion

For a given diffracted wavelength I in order m (which corresponds to an angle of diffraction \mathbf{b}), the *linear dispersion* of a grating system is the product of the angular dispersion D and the effective focal length $r'(\mathbf{b})$ of the system:

$$r' D = r' \frac{db}{dI} = \frac{mr'}{d \cos \mathbf{b}} = \frac{mr'}{d} \sec \mathbf{b} = Gmr' \sec \mathbf{b}. \quad (2-16)$$

The quantity $r' \Delta \mathbf{b} = \Delta l$ is the change in position along the spectrum (a real distance, rather than a wavelength). We have written $r'(\mathbf{b})$ for the focal length to

show explicitly that it may depend on the diffraction angle \mathbf{b} (which, in turn, depends on \mathbf{D}).

The *reciprocal linear dispersion*, sometimes called the *plate factor* P , is more often considered; it is simply the reciprocal of $r' D$, usually measured in nm/mm:

$$P = \frac{d \cos \mathbf{b}}{mr'}. \quad (2-14')$$

P is a measure of the change in wavelength (in nm) corresponding to a change in location along the spectrum (in mm). It should be noted that the terminology *plate factor* is used by some authors to represent the quantity $1/\sin \mathbf{F}$, where \mathbf{F} is the angle the spectrum makes with the line perpendicular to the diffracted rays (see Figure 2-6); in order to avoid confusion, we call the quantity $1/\sin \mathbf{F}$ the *obliquity factor*. When the image plane for a particular wavelength is not perpendicular to the diffracted rays (*i.e.*, when $\mathbf{F} \neq 90^\circ$), P must be multiplied by the obliquity factor to obtain the correct reciprocal linear dispersion in the image plane.

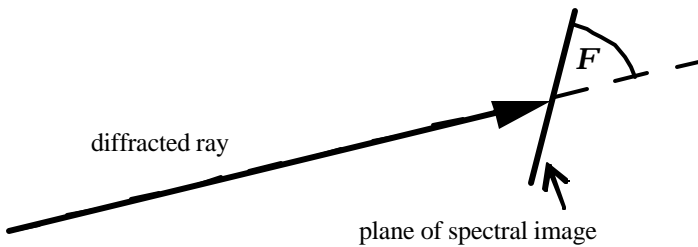


Figure 2-6. The obliquity angle \mathbf{F} . The spectral image recorded need not lie in the plane perpendicular to the diffracted ray (*i.e.*, $\mathbf{F} \neq 90^\circ$).

2.4. RESOLVING POWER, SPECTRAL RESOLUTION, AND BANDPASS

2.4.1. Resolving power

The resolving power R of a grating is a measure of its ability to separate adjacent spectral lines of average wavelength λ . It is usually expressed as the dimensionless quantity

$$R = \frac{\lambda}{\Delta\lambda}. \quad (2-17)$$

Here $\Delta\lambda$ is the *limit of resolution*, the difference in wavelength between two lines of equal intensity that can be distinguished (that is, the peaks of two wavelengths λ_1 and λ_2 for which the separation $|\lambda_1 - \lambda_2| < \Delta\lambda$ will be ambiguous). Often the *Rayleigh criterion* is used to determine $\Delta\lambda$ – that is, the intensity maxima of two neighboring wavelengths are resolvable (*i.e.*, identifiable as distinct spectral lines) if the intensity maximum of one wavelength coincides with the intensity minimum of the other wavelength.⁶

The theoretical resolving power of a planar diffraction grating is given in elementary optics textbooks as

$$R = mN, \quad (2-18)$$

where m is the diffraction order and N is the total number of grooves illuminated on the surface of the grating. For negative orders ($m < 0$), the absolute value of R is considered.

A more meaningful expression for R is derived below. The grating equation can be used to replace m in Eq. (2-18):

$$R = \frac{Nd(\sin \mathbf{a} + \sin \mathbf{b})}{\lambda}. \quad (2-19)$$

⁶ D. W. Ball, *The Basics of Spectroscopy*, SPIE Press (2001), ch. 8.

If the groove spacing d is uniform over the surface of the grating, and if the grating substrate is planar, the quantity Nd is simply the ruled width W of the grating, so

$$R = \frac{W(\sin \mathbf{a} + \sin \mathbf{b})}{\mathbf{l}}. \quad (2-20)$$

As expressed by Eq. (2-20), R is not dependent explicitly on the spectral order or the number of grooves; these parameters are contained within the ruled width and the angles of incidence and diffraction. Since

$$|\sin \mathbf{a} + \sin \mathbf{b}| < 2, \quad (2-21)$$

the maximum attainable resolving power is

$$R_{\text{MAX}} = \frac{2W}{\mathbf{l}}, \quad (2-22)$$

regardless of the order m or number of grooves N under illumination. This maximum condition corresponds to the grazing Littrow configuration, *i.e.*, $|\mathbf{a}| \sim 90^\circ$ (grazing incidence) and $\mathbf{a} \sim \mathbf{b}$ (Littrow).

It is useful to consider the resolving power as being determined by the maximum phase retardation of the extreme rays diffracted from the grating.⁷ Measuring the difference in optical path lengths between the rays diffracted from opposite sides of the grating provides the maximum phase retardation; dividing this quantity by the wavelength \mathbf{l} of the diffracted light gives the resolving power R .

The degree to which the theoretical resolving power is attained depends not only on the angles \mathbf{a} and \mathbf{b} , but also on the optical quality of the grating surface, the uniformity of the groove spacing, the quality of the associated optics in the system, and the width of the slits (or detector elements). Any departure of the diffracted wavefront greater than $\mathbf{l}/10$ from a plane (for a plane grating) or from a sphere (for a spherical grating) will result in a loss of resolving power due to aberrations at the image plane. The grating groove spacing must be kept

⁷ N. Abramson, "Principle of least wave change," *J. Opt. Soc. Am.* **A6**, 627-629 (1989).

constant to within about one percent of the wavelength at which theoretical performance is desired. Experimental details, such as slit width, air currents, and vibrations can seriously interfere with obtaining optimal results.

The practical resolving power is limited by the spectral width of the spectral lines emitted by the source. For this reason, systems with resolving powers greater than $R = 500,000$ are not usually required except for the study of spectral line shapes, Zeeman effects, and line shifts, and are not needed for separating individual spectral lines.

A convenient test of resolving power is to examine the isotopic structure of the mercury emission line at $\lambda = 546.1 \text{ nm}$ (see Section 11.4). Another test for resolving power is to examine the line profile generated in a spectrograph or scanning spectrometer when a single mode laser is used as the light source. The full width at half maximum intensity (FWHM) can be used as the criterion for $\Delta\lambda$. Unfortunately, resolving power measurements are the convoluted result of all optical elements in the system, including the locations and dimensions of the entrance and exit slits and the auxiliary lenses and mirrors, as well as the quality of these elements. Their effects on resolving power measurements are necessarily superimposed on those of the grating.

2.4.2. Spectral resolution

While resolving power can be considered a characteristic of the grating and the angles at which it is used, the ability to resolve two wavelengths λ_1 and $\lambda_2 = \lambda_1 + \Delta\lambda$ generally depends not only on the grating but on the dimensions and locations of the entrance and exit slits (or detector elements), the aberrations in the images, and the magnification of the images. The minimum wavelength difference $\Delta\lambda$ (also called the *limit of resolution*, or simply *resolution*) between two wavelengths that can be resolved unambiguously can be determined by convoluting the image of the entrance aperture (at the image plane) with the exit aperture (or detector element). This measure of the ability of a grating system to resolve nearby wavelengths is arguably more relevant than is resolving power, since it takes into account the image effects of the system. While resolving power is a dimensionless quantity, resolution has spectral units (usually nanometers).

2.4.3. Bandpass

The (*spectral*) *bandpass* B of a spectroscopic system is the wavelength interval of the light that passes through the exit slit (or falls onto a detector element). It is often defined as the difference in wavelengths between the points of half-maximum intensity on either side of an intensity maximum.

For an optical system in which the width of the image of the entrance slit is roughly equal to the width of the exit slit, an estimate for bandpass is the product of the exit slit width w' and the reciprocal linear dispersion P :

$$B \sim w' P. \quad (2-23)$$

An instrument with smaller bandpass can resolve wavelengths that are closer together than an instrument with a larger bandpass. Bandpass can be reduced by decreasing the width of the exit slit (to a certain limit; see Chapter 8), but usually at the expense of decreasing light intensity as well.

See Section 8.3 for additional comments on instrumental bandpass.

2.4.4. Resolving power vs. resolution

In the literature, the terms *resolving power* and *resolution* are sometimes interchanged. While the word *power* has a very specific meaning (energy per unit time), the phrase *resolving power* does not involve *power* in this way; as suggested by Hutley, though, we may think of resolving power as “ability to resolve”.⁸

The comments above regarding resolving power and resolution pertain to planar classical gratings used in collimated light (plane waves). The situation is complicated for gratings on concave substrates or with groove patterns consisting of unequally spaced lines, which restrict the usefulness of the previously defined simple formulas, though they may still yield useful approximations. Even in these cases, though, the concept of maximum retardation is still a useful measure of the resolving power, and the convolution of the image and the exit slit is still a useful measure of resolution.

⁸ M. C. Hutley, *Diffraction Gratings*, Academic Press (New York, New York: 1982), p. 29.

2.5. FOCAL LENGTH AND f /NUMBER

For gratings (or grating systems) that image as well as diffract light, or disperse light that is not collimated, a *focal length* may be defined. If the beam diffracted from a grating of a given wavelength λ and order m converges to a focus, then the distance between this focus and the grating center is the focal length $r'(\lambda)$. [If the diffracted light is collimated, and then focused by a mirror or lens, the focal length is that of the refocusing mirror or lens and not the distance to the grating.] If the diffracted light is diverging, the focal length may still be defined, although by convention we take it to be negative (indicating that there is a virtual image behind the grating). Similarly, the incident light may diverge toward the grating (so we define the incidence or entrance slit distance $r(\lambda) > 0$) or it may converge toward a focus behind the grating (for which $r(\lambda) < 0$). Usually gratings are used in configurations for which r does not depend on wavelength (though in such cases r' usually depends on λ).

In Figure 2-7, a typical concave grating configuration is shown; the monochromatic incident light (of wavelength λ) diverges from a point source at A and is diffracted toward B. Points A and B are distances r and r' , respectively, from the grating center O. In this figure, both r and r' are positive.

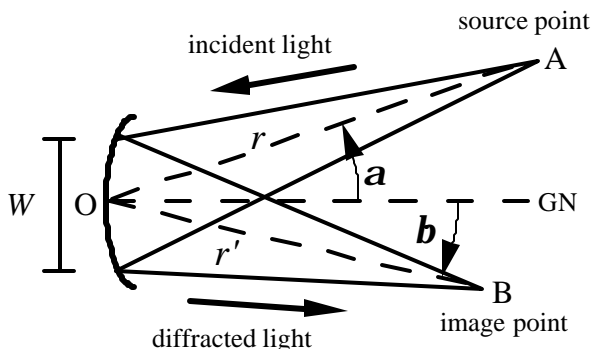


Figure 2-7. Geometry for focal distances and focal ratios (f /numbers). GN is the grating normal (perpendicular to the grating at its center, O), W is the width of the grating (its dimension perpendicular to the groove direction, which is out of the page), and A and B are the source and image points, respectively.

Calling the width (or diameter) of the grating (in the dispersion plane) W allows the *input* and *output* f /numbers (also called *focal ratios*) to be defined:

$$f/\text{no}_{\text{INPUT}} = \frac{r}{W}, \quad f/\text{no}_{\text{OUTPUT}} = \frac{r'(\mathbf{l})}{W}. \quad (2-24)$$

Usually the input f /number is matched to the f /number of the light cone leaving the entrance optics (*e.g.*, an entrance slit or fiber) in order to use as much of the grating surface for diffraction as possible. This increases the amount of diffracted energy while not overfilling the grating (which would generally contribute to instrumental stray light; see Chapter 10).

For oblique (non-normal) incidence or diffraction, Eqs. (2-25) are often modified by replacing W with the projected width of the grating:

$$f/\text{no}_{\text{INPUT}} = \frac{r}{W \cos \mathbf{a}}, \quad f/\text{no}_{\text{OUTPUT}} = \frac{r'(\mathbf{l})}{W \cos \mathbf{b}}. \quad (2-25)$$

These equations account for the reduced width of the grating as seen by the entrance and exit slits; moving toward oblique angles (*i.e.*, increasing $|\mathbf{a}|$ or $|\mathbf{b}|$) decreases the projected width and therefore increases the f /number.

The focal length is an important parameter in the design and specification of grating spectrometers, since it governs the overall size of the optical system (unless folding mirrors are used). The ratio between the input and output focal lengths determines the projected width of the entrance slit that must be matched to the exit slit width or detector element size. The f /number is also important, as it is generally true that spectral aberrations decrease as f /number increases. Unfortunately, increasing the input f /number results in the grating subtending a smaller solid angle as seen from the entrance slit; this will reduce the amount of light energy the grating collects and consequently reduce the intensity of the diffracted beams. This trade-off prohibits the formulation of a simple rule for choosing the input and output f /numbers, so sophisticated design procedures have been developed to minimize aberrations while maximizing collected energy. See Chapter 7 for a discussion of the imaging properties and Chapter 8 for a description of the efficiency characteristics of grating systems.

2.6. ANAMORPHIC MAGNIFICATION

For a given wavelength λ , we may consider the ratio of the width of a collimated diffracted beam to that of a collimated incident beam to be a measure of the effective magnification of the grating (see Figure 2-8). From this figure we see that this ratio is

$$\frac{b}{a} = \frac{\cos \theta}{\cos \alpha} \quad (2-26)$$

Since α and θ depend on λ through the grating equation (2-1), this magnification will vary with wavelength. The ratio b/a is called the *anamorphic magnification*; for a given wavelength λ , it depends only on the angular configuration in which the grating is used.

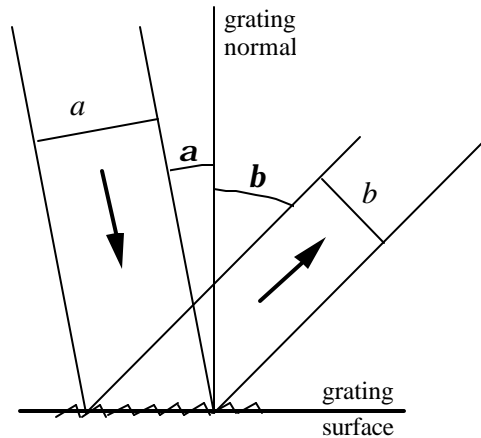


Figure 2-8. *Anamorphic magnification.* The ratio b/a of the beam widths equals the anamorphic magnification; the grating equation (2-1) guarantees that this ratio will not equal unity unless $m = 0$ (specular reflection) or $\alpha = \theta$ (the Littrow configuration).

The magnification of an object not located at infinity (so that the incident rays are not collimated) is discussed in Chapter 8.

2.7. FREE SPECTRAL RANGE

For a given set of incidence and diffraction angles, the grating equation is satisfied for a different wavelength for each integral diffraction order m . Thus light of several wavelengths (each in a different order) will be diffracted along the same direction: light of wavelength I in order m is diffracted along the same direction as light of wavelength $I/2$ in order $2m$, etc.

The range of wavelengths in a given spectral order for which superposition of light from adjacent orders does not occur is called the *free spectral range* F_1 . It can be calculated directly from its definition: in order m , the wavelength of light that diffracts along the direction of I in order $m+1$ is $I + \Delta I$, where

$$I + \Delta I = \frac{m+1}{m} I, \quad (2-27)$$

from which

$$F_1 = \Delta I = \frac{I}{m}. \quad (2-28)$$

The concept of free spectral range applies to all gratings capable of operation in more than one diffraction order, but it is particularly important in the case of echelles, because they operate in high orders with correspondingly short free spectral ranges.

Free spectral range and order sorting are intimately related, since grating systems with greater free spectral ranges may have less need for filters (or cross-dispersers) that absorb or diffract light from overlapping spectral orders. This is one reason why first-order applications are widely popular.

2.8. ENERGY DISTRIBUTION (GRATING EFFICIENCY)

The distribution of power of a given wavelength diffracted by a grating into the various spectral order depends on many parameters, including the power and polarization of the incident light, the angles of incidence and diffraction, the (complex) index of refraction of the materials at the surface of the grating, and the groove spacing. A complete treatment of grating efficiency requires the vector

formulation of electromagnetic theory (*i.e.*, Maxwell's equations) applied to corrugated surfaces, which has been studied in detail over the past few decades. While the theory does not yield conclusions easily, certain rules of thumb can be useful in making approximate predictions.

The simplest and most widely used rule of thumb regarding grating efficiency (for reflection gratings) is the *blaze condition*

$$m\lambda = 2d\sin q_B, \quad (2-29)$$

where q_B (often called the *blaze angle* of the grating) is the angle between the face of the groove and the plane of the grating (see Figure 2-9). When the blaze condition is satisfied, the incident and diffracted rays follow the law of reflection when viewed from the facet; that is, we have

$$a - q_B = b - q_B. \quad (2-30)$$

Because of this relationship, it is often said that when a grating is used at the blaze condition, the facets act as tiny mirrors – this is not strictly true (since the facet “mirror” is roughly of the same dimensions as the wavelength itself, ray optics does not provide an adequate physical model), but it is a useful way to remember the conditions under which a grating can be used to enhance efficiency.

Eq. (2-29) generally leads to the highest efficiency when the following condition is also satisfied:

$$2K = a - b = 0, \quad (2-31)$$

where $2K$ was defined above as the angle between the incident and diffracted beams (see Eq. (2-6)). Eqs. (2-29) and (2-31) collectively define the *Littrow blaze condition*. When Eq. (2-31) is not satisfied (*i.e.*, $a \neq b$ and therefore the grating is not used in the Littrow configuration), efficiency is generally seen to decrease as one moves further off Littrow (*i.e.*, as $|2K|$ increases).

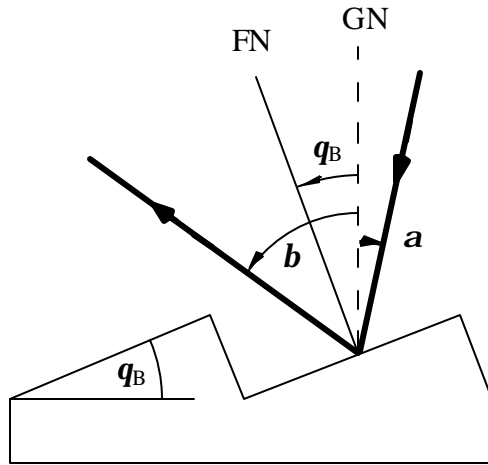


Figure 2-9. *Blaze condition.* The angles of incidence a and diffraction b are shown in relation to the facet angle q_B for the blaze condition. GN is the grating normal and FN is the facet normal. When the facet normal bisects the angle between the incident and diffracted rays, the blaze condition (Eq. (2-29)) is satisfied.

For a given blaze angle q_B , the Littrow blaze condition provides the *blaze wavelength* I_B , the wavelength for which the efficiency is maximal when the grating is used in the Littrow configuration:

$$I_B = \frac{2d}{m} \sin q_B, \quad \text{in Littrow.} \quad (2-32)$$

Many grating catalogs specify the *first-order Littrow blaze wavelength* for each grating:

$$I_B = 2d \sin q_B, \quad \text{in Littrow } (m = 1). \quad (2-33)$$

Unless a diffraction order is specified, quoted values of I_B are generally assumed to be for the first diffraction order, in Littrow.

Recently, computer codes have become commercially available that accurately predict grating efficiency for a wide variety of groove profiles over wide spectral ranges.

The topic of grating efficiency is addressed more fully in Chapter 9.

2.9. SCATTERED AND STRAY LIGHT

All light that reaches the detector of a grating-based instrument from anywhere other than the grating, by any means other than diffraction as governed by Eq. (2-1), for any order other than the primary diffraction order of use, is called *instrumental stray light* (or more commonly, simply *stray light*). All components in an optical system contribute stray light, as will any baffles, apertures, and partially reflecting surfaces. Unwanted light originating from an illuminated grating itself is often called *scattered light* or *grating scatter*.

Instrumental stray light can introduce inaccuracies in the output of an absorption spectrometer used for chemical analysis. These instruments usually employ a “white light” (broad spectrum) light source and a monochromator to isolate a narrow spectral range from the white light spectrum; however, some of the light at other wavelengths will generally reach the detector, which will tend to make an absorbance reading too low (*i.e.*, the sample will seem to be slightly more transmissive than it would in the absence of stray light). In most commercial benchtop spectrometers, such errors are on the order of 0.1 to 1 percent (and can be much lower with proper instrument design) but in certain circumstances (*e.g.*, in Raman spectroscopy), instrumental stray light can lead to significant errors. Grating scatter and instrumental stray light are addressed in more detail in Chapter 10.

2.10. SIGNAL-TO-NOISE RATIO (SNR)

The *signal-to-noise ratio* (SNR) is the ratio of diffracted energy to unwanted light energy. While we might be tempted to think that increasing diffraction efficiency will increase SNR, stray light usually plays the limiting role in the achievable SNR for a grating system.

Replicated gratings from ruled master gratings generally have quite high SNRs, though holographic gratings sometimes have even higher SNRs, since

they have no ghosts due to periodic errors in groove location and lower interorder stray light.

As SNR is a property of the optical instrument, not of the grating only, there exist no clear rules of thumb regarding what type of grating will provide higher SNR.

Excerpt from Diffraction Grating Handbook -
Copyright 2005 Newport Corporation
Email: gratings.sales@newport.com to receive a complete copy.