Size and Spectrum

Bigger isn't necessarily better when you're trying to choose a monochromator or spectrograph to analyze chemicals, colors and communications channels.

by Jean-Luc Domanchin and John R. Gilchrist

Photonics is increasingly influencing our lives, even if many people do not realize it. For example, fields such as semiconductor, chemical, food and color analysis; light source and pollution measurement; medical diagnostics; and telecommunications use monochromators or spectrographs during their processing, certification or regulatory testing.

Nonexpert users can find it difficult to compare different monochromator systems to choose the most suitable spectroscopic configuration for an application. They often misunderstand specifications such as dispersion, precision, image quality and stray light.

Users prefer to talk about "small" and "large" monochromators: those with focal lengths ≤0.3 m or those larger than 0.3 m. The implication is that large monochromators are better. In some cases, this assumption is correct, but in many others, it is not. Each application has its own performance requirements, and users must often make difficult price/performance trade-offs in choosing the best instrument configuration.

Monochromators and spectrographs are the most widely used dispersive instruments in spectroscopy. They use dispersive elements, such as prisms or diffraction gratings, and image-transfer optics to separate small wavelengths from a polychromatic source.

Detectors for monochromators are usually single-channel, large-area devices. Spectrographs use a fixed grating geometry to monitor a spectral range dispersed over a linear array of multiple detector elements. Few manufacturers offer prism-based monochromators. Grating-based monochromators and spectrographs, however, are available in a wide variety of configurations, most commonly for use in the 10-nm to 20-µm wavelength range.

Multislit source

A diffraction grating is a plane or concave element with closely spaced grooves. When illuminated by collimated radiation, the grating acts as a multislit source, diffracting different wavelengths that constructively interfere at different angles. Most modern spectrometers use reflection gratings with groove densities from 75 to 3600 grooves per millimeter, depending upon the spectral range and resolution required.

Grating types are categorized by their method of production: ruled or holographic. Ruled gratings are made by replication from a master grating prepared by a high-precision ruling engine. Holographic gratings are made by projecting an interference pattern onto a photoresist plate, developing this to produce the pattern and then etching it into the glass for permanence. Holographic gratings have essentially perfect groove patterns and significantly better stray-light rejection than ruled gratings, and are almost totally free of false lines or ghosts. However, they also have a slightly lower reflection efficiency.

One of the most common monochromator configurations is the Czerny-Turner configuration (Figure 1). Many other designs are available, but all follow the same oper-

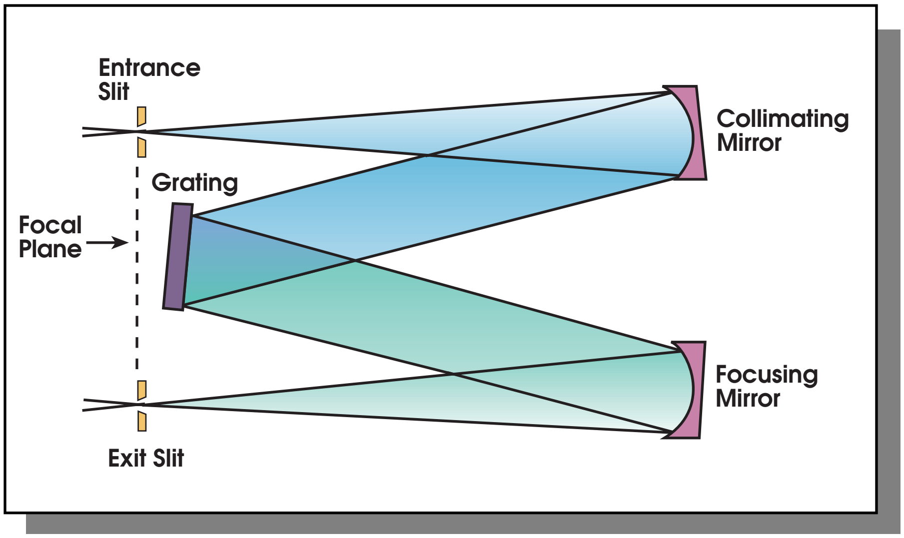

Figure 1. *Monochromator configurations, like this Czerny-Turner design, follow a similar operating principle: Light passes through a slit and reflects off a collimating mirror to a diffraction grating, which separates the spectrum. A focusing mirror reflects the diffracted light onto the exit slit.*

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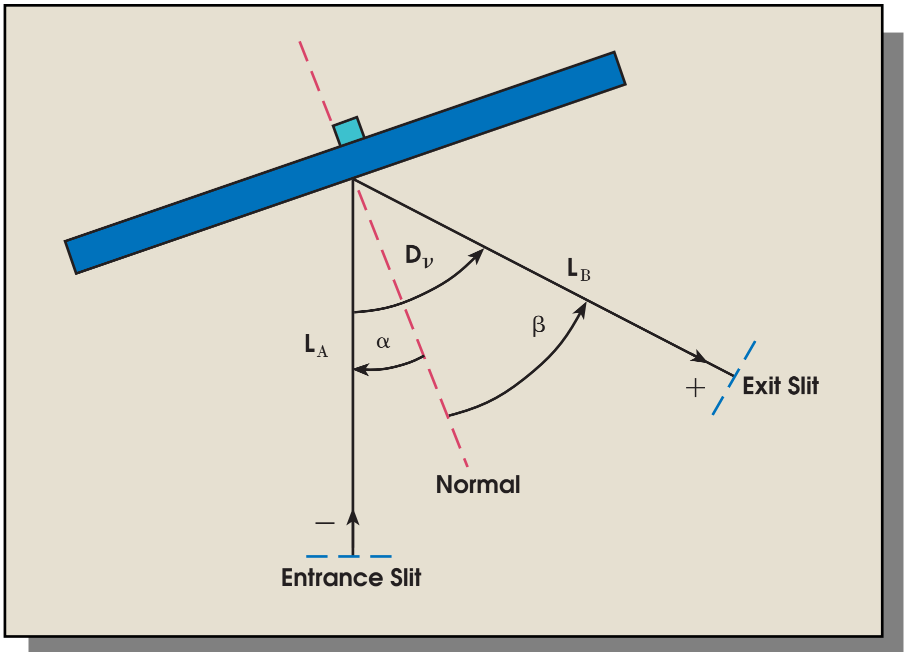

Figure 2. *Rotating the diffraction grating position scans the wavelengths across the monochromator's exit slit. The accuracy and speed of the rotation depend on the grating motor drive, with sine bar mechanisms providing excellent accuracy and repeatability at the cost of speed.*

ating principle: The incident light passes through the entrance slit and hits a collimating mirror that produces a parallel polychromatic light beam onto the diffraction grating. The grating spatially separates the spectrum of the incident light, and the focusing mirror reflects the diffracted light onto the exit slit. Each wavelength is incident upon the exit plane at a specific angle. Rotating the grating position scans the wavelengths across the exit slit, discriminating between each wavelength.

The grating equation specifies the angle that is required to bring each wavelength through the exit slit (Figure 2).

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

where k is the diffraction order, n the grating groove density and λ the vacuum wavelength in nanometers.

The slits play an important role in determining the spectral resolution and throughput of the monochromator. In most cases, they are adjustable and can vary from a few microns to several millimeters in width. Generally, the exit and entrance slits are the same width.

Several characteristics are of importance in a monochromator.

The linear dispersion is how far apart, spatially, two wavelengths are in the focal plane, $D_L = dx/d\lambda$. The more commonly quoted figure is the reciprocal linear dispersion, $R_D = D_L^{-1} = d\lambda/dx$, which represents the wavelength range within a unit distance in the focal plane.

The instrument's limiting aperture — often the diffraction grating — determines the *f* number and solid angle. With a limiting aperture diameter of *L*, a projected area of *A* and focal length of the collimating mirror of *F*, the *f* number is approximately equal to F/L. The solid angle is then $\Omega = A/F^2 = \pi/[4(f/\#)^2]$.

The spectral bandpass is the half-width of the wavelengths that pass across the exit slit. The spectral bandpass for a given slit width, *W*, is $S_\lambda = R_D W$, except at very small slit widths, where diffraction effects and aberrations come into play. Thus, reducing the slit widths will usually decrease the bandpass.

The monochromator's resolution relates closely to its spectral dispersion. The dispersion governs how far apart two wavelengths are, while the resolution specifies whether the separation can be distinguished. The Rayleigh criterion states that two wavelengths, λ_1 and λ_2, are resolved if the central maximum of one line falls on a diffraction minimum of the other (Figure 3). Thus, the spectral resolution can be defined by $\Delta\lambda = \bar{\lambda}/(D_\alpha W)$, where $\bar{\lambda}$ is the average wavelength between the two lines and D_α is the system's angular dispersion.

Stray light is any radiation that the monochromator passes outside the selected spectral position and bandpass. In many cases, the specification of stray light is made by reference to the relative amount of radiation being passed at the spectral position defined as an integer number of bandpass values from the test source — often a laser line.

For example, a typical measurement involves just filling the grating of a monochromator, then measuring intensity at the laser wavelength and at another wavelength, eight bandpasses away. The ratio of the latter to the former is the stray light of the system under this criterion. Typically, stray light is very difficult to measure because it strongly depends upon the wavelength, the bandpass used and the type of source.

The optical throughput of a monochromator depends upon the source, the slit height, the collected solid angle, the transmission factor of the optics and the convolution of the entrance and exit slit widths. The light-gathering capacity is defined by:

$$LGC = \frac{height_{slit}\ \text{(mm)}}{(f/\#)^2 \times dispersion\ \text{(nm/mm)}}$$

Top criteria:
Dispersion, resolution, bandpass

The dispersion shows the capability to disperse light. It gives the usable bandpass of a monochromator or indicates the spectral range of a spectrograph equipped with a multichannel array detector such as a CCD camera or InGaAs array. Changing the width of the slit aperture can adjust the bandpass.

Spectral resolution is inversely proportional to the linear dispersion of a monochromator. The resolution requirement of the experiment is often the key performance requirement of any application. For narrow structure analysis (resolution better than 0.1 nm in the visible range), large monochromators are the best choice because they offer increased spectral dispersion and thus a higher spectral resolution.

If the application's most important requirement is to acquire a large spectral range in one shot, small spectrographs are better, as in a process application. In fact, single monochromators with a focal length below 0.3 m are suitable for most applications where the influence of stray light is not considered a major problem.

Laboratory researchers who don't need high resolution and wide range at the same time, however, should choose larger spectrographs. These users can change gratings (i.e., to a higher or lower groove density) or acquire multiple spectra to achieve complete results.

Second criteria: Accuracy, speed

Monochromators work by scanning through the spectral features of the optical signals, step by step. As a result, the measurement process is generally slower than that of spectrographs with multichannel array detectors that operate in a fixed grating position and directly acquire a full spectrum according to their dispersion.

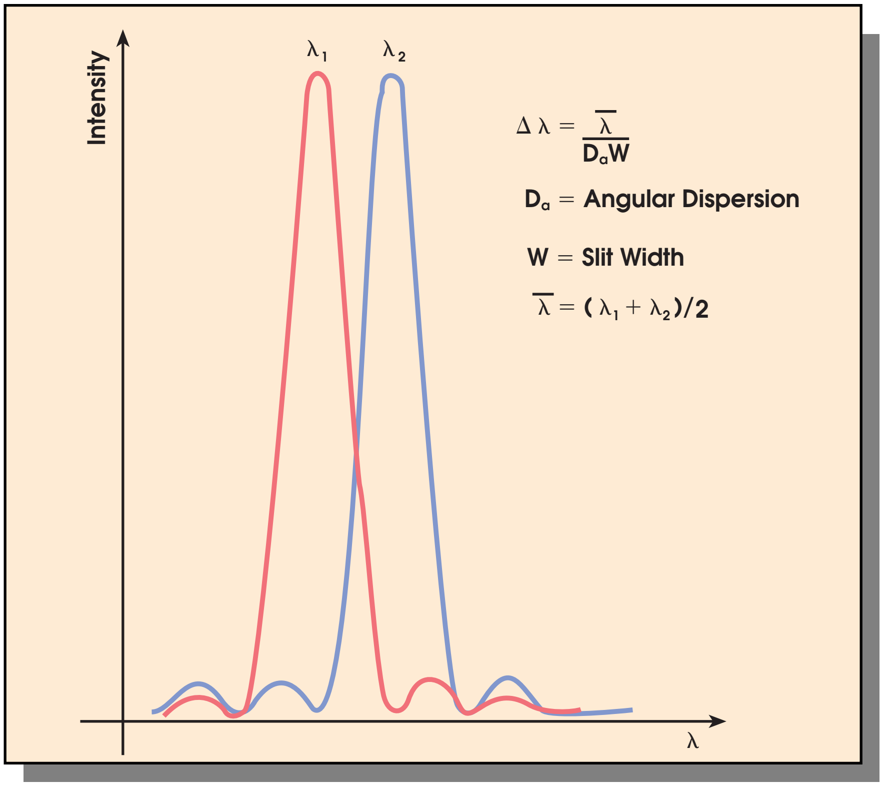

Figure 3. *A monochromator's resolution specifies whether the instrument can distinguish between two wavelengths. This parameter is closely related to the instrument's spectral dispersion.*

However, accuracy and speed depend mainly on the grating motor drive. Instruments with 0.5-m or higher focal length are usually equipped with sine bar mechanisms that give excellent accuracy (better than 0.1 nm) and repeatability (better than 0.01 nm). But the trade-off is speed: It can take several minutes to scan a large spectral range with high spectral resolution in monochromator mode.

Monochromator: An instrument that separates one wavelength or bandpass from a polychromatic source. Scanning monochromators can sequentially scan a range of wavelengths or bands.

Spectrometer: An instrument that measures the distribution of radiation from a broadband source. Its principal components are a monochromator and a radiant power detector such as a silicon detector, a photomultiplier tube or other single detector.

Spectrograph: An instrument that presents a range of wavelengths at the exit focal plane for detection by an array detector. Many modern spectrographs have two exits, one with an exit slit, so that one instrument can serve as both a spectrograph and a scanning monochromator.

Bandpass: The width of the spectrum that a monochromator passes when illuminated by a light source with a continuous spectrum. Usually bandpass decreases with slit width.

Focal length: The distance from the exit-imaging mirror to the flat focal plane. Increasing the focal length usually increases resolution and reduces the bandpass.

***f* number (*f*/#):** The input aperture of the monochromator. It measures the ability of a device to collect radiation in the entrance slit: The light-gathering power of an optical device increases as the inverse square of the *f* number.

Smaller devices commonly use direct or worm drives because their resolution specifications are lower. In this case, they set the grating position within a few seconds.

Third criteria: Throughput, imaging quality

Most of the time, small monochromators and spectrographs have better throughput than large ones because of their larger numerical apertures (*f* numbers) and simpler design (often with fewer optical components).

However, the numerical aperture is not the final consideration in optical throughput. The linear dispersion is also important because it defines the input aperture sizes for a particular spectral resolution.

A more useful figure of merit for comparing monochromators for imaging applications is light-gathering capability. Manufacturers of small instruments usually find that to preserve spectral resolution, they can produce only a small image. Producing a larger image, especially across a large spectral range, is very difficult because of the spatial corrections required.

The commercial introduction of imaging spectrographs has partially corrected the spatial imaging quality issues. These instruments use toroidal gratings or toroidal mirrors to correct for astigmatism in the image plane and to improve image quality while keeping the numerical aperture at the same level as nonimaging devices. This correction requires complex calculations. The choice of the toroid, the optical incident angles of the device and wavelength optimizations shows the knowledge of the manufacturer.

Well-corrected, fixed, compact spectrographs can provide excellent image quality. Some can discriminate three or four spectral channels over a 6-mm-tall focal plane. Interesting axial spectrograph configurations using grisms and lenses also offer excellent image quality over a few hundred nanometers in the visible range.

Some 30-cm or larger imaging spectrographs allow more than 10-channel analysis with a minimized channel overlap.

Final criteria: Stray light, design, focal length

Stray light relates mainly to the quality of the device's optical components (mirrors and grating). The user is generally not aware of stray light or improper internal reflection, which can produce poor results.

Because of their slit/slit configuration, monochromators have less stray light or re-entrant light than do spectrographs, which have no exit slit. However, when the stray light is important in an application, large-focal-length instruments or double monochromators are the best choice. Small devices present more risk of stray light than larger ones.

In terms of optical design, most large monochromators/spectrographs use the asymmetric Czerny-Turner configuration. Smaller instruments tend to use an asymmetric "V" configuration as a compromise.

Weighing the trade-offs

No one device can cover all spectroscopic applications. However, a user who carefully analyzes the spectral and performance requirements of an application can weigh the tradeoffs involved in choosing between small- and large-focal-length monochromators and spectrographs.

If you need to analyze a short spectral range at low resolution, you can probably use an inexpensive, compact monochromator or spectrograph. Even if these devices have stray light, chemometric calibration methods can correct it without influencing the results.

However, if you need high resolution, accuracy or versatility, large monochromators and spectrographs are often the safest buy. That is why these are generally the best instruments for research or high-technology industries. ☐

Meet the authors

Jean-Luc Domanchin is manager of spectroscopy systems at Jobin Yvon Inc. in Edison, N.J. He has a degree in optics.

John R. Gilchrist is director of the Optical Spectroscopy Div. of Jobin Yvon. He graduated from Strathclyde University in Glasgow, UK.