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Direct Digital Drive for Digikrom Products - Simple, Rugged, Reliable

In 1987 SP Laser introduced the first change in grating drives in more than 50 years. Using digital electronics, SP replaced the unreliable mechanical linkages that were used to translate the rotary motion of the drive motor into the sine motion needed for wavelength linearity. Photo 1 shows a typical direct drive grating table that SP manufactures. SP named this method Direct Digital Drive and incorporated it into a new line of Digikrom monochromators and spectrographs.

The equation relating grating angle ($\Theta$) and wavelength ($\lambda$) is the well known non-linear equation,

$$m\lambda=2dsin\theta cos\phi/2$$

where $\phi$ is the angle between the central incident ray and the central exiting ray that reaches the exit slit, and $\Theta$ is the grating rotation from zero order.

In a spectrometer the rotary motion of the drive motor and associated reduction gears linearly determines theta. In sine-drive instruments a second mechanism, a cam or a sine arm, creates the sine function.

SP Laser replaced the mechanical sine mechanism with digital electronic calculation of sine (theta). When a wavelength is input to a Digikrom monochromator, the internal microprocessor calculates the required sine (theta) and the corresponding angle theta. In about 500 microseconds this calculation finds the number of stepping motor steps required to reach the angle corresponding to the wavelength. This would not have been possible without the microprocessor revolution that permits inclusion of a micro-controller within each instrument at a reasonable cost.

The advantages of Direct Digital Drive are significant. The mechanical mechanism is simpler and more reliable. Calibration is easier and more accurate. A multi-grating turret with automatic grating change becomes a simple, inexpensive option. Finally, inclusion of a micro-controller with each spectrometer makes computer control of the spectrometer easy. These advantages come with a price reduction because of the replacement of expensive mechanical parts with inexpensive, reliable electronics.

Both Direct Digital Drives and conventional sine drives use a stepping motor, which typically rotates 0.9 degrees per step. The stepper motor rotation is reduced via gear reduction. But, at this point the traditional sine-drive becomes complex.

In the traditional sine-drive, the gear reduction is typically a 5:1 worm and wheel. This output then rotates a lead screw that moves a nut along the opposite side of a right triangle. A precision slide is needed to prevent the nut from rotating as it translates. A hypotenuse arm pivots around the axis of rotation of the grating to follow the nut. As the arm pivots, it rotates the grating proportional to the sine of the angle.

In Direct Digital Drive, a 120:1 worm and wheel gear reduction connects the stepping motor directly to the rotational shaft of the grating. No other mechanism is necessary. Only a single precision worm and wheel is used. There are fewer parts to wear or break and no tolerance errors accumulate as in cascaded mechanisms.

Calibration is easier with the Direct Digital Drive. Only two points - the slope
and intercept - need to be specified to calibrate the grating equation. The intercept is optical zero; at optical zero, theta is zero, m is zero, the grating acts like a mirror, and the spectrometer transmits white light. The slope, \(2 \cos \phi / 2\) is found from the angle \(\theta\) at a known wavelength.

In the traditional sine drive it is quite difficult to make the mechanical zero of the sine function mechanism equal to the optical zero. While optical zero can be determined precisely as the point of specular reflection, the mechanical zero can only be determined with mechanical gauges or complicated calculations derived from the errors at multiple calibration wavelengths. In fact, a separate rotational adjustment is needed on each grating in a sine-drive system to make the mechanical and optical zeros coincide.

In Direct Digital Drive, the sine function is electronic, and the electronic sine function is reset to begin at the optical zero. The correspondence between the optical zero and the zero of the sine function is then exact. When power is applied to a SP Spectrometer, a predetermined position in the mechanical rotation - the home position - is detected. The grating then rotates to optical zero. The offset angle between home and optical zero has been previously stored in the microprocessor memory. If the optical zero is incorrect - for example, if gratings were changed - the user commands further grating rotation until optical zero is identified. The micro-controller remembers the new offset angle. Calibration is thus simple and exact.

Direct Digital Drive also allows the option of a multiple grating turret with automatic grating change, see Photo 1. This is a tremendous advantage when a wide spectral range needs to be covered because the entire range can be studied without disassembling, realigning and recalibrating the spectrometer to replace gratings.

The worm and wheel mechanism allows 360° rotation of the grating turret, so it is possible to have two or more gratings on the same turret. This is not possible with the traditional sine-drive, which is limited to about 70 degrees of total rotation. Direct Digital Drive makes the multiple grating turret simple and inexpensive.

In addition, with proper design of the dual or triple grating turret, no vignetting results from the translation on the front face of the grating as it rotates around the central axis. The final enhancement of the Direct Digital Drive is the additional capacity inherent in including a micro-controller in the spectrometer. The included micro-controller allows a simple interface, motorized slit control and automatic grating change at little additional cost. The simple interface is the biggest advantage. It is now unnecessary for the user to build a stepper motor interface or to buy additional motor drive boxes. The micro-controllers in Digikrom spectrometers accept simple commands over an RS232C serial interface from any computer.

The advantages of Direct Digital Drive are clear. The mechanics are simple and more reliable. Calibration is easier and more accurate. A multi-grating turret with automatic grating change is a simple, inexpensive option. Inclusion of a micro-controller with each spectrometer makes computer control easy. Finally, with expensive mechanics replaced by low cost electronics, the price is less.
Subtractive Dispersion Spectrometers

When we think of a spectrometer we envision white light entering and being dispersed by a prism or grating and exiting in a dispersed spectrum across an arc. This is the archetype of spectral dispersion. If we reverse this process, an arc of color enters the prism or grating and a homogenous white light exits. This reversal is called spectral recombination. When we couple this spectral dispersion followed by spectral recombination we have created an optical curiosity called subtractive dispersion. Today, time-resolved spectroscopy and imaging applications are reviving interest in this technique. (Figure 1) Two Digikrom models, the DK242 and the CM112, employ it.

A simple subtractive dispersion monochromator appears in the figure at right. The instrument consists of coupled grating monochromators. White light enters the entrance of the first monochromator and is dispersed across the shared intermediate slit. The intermediate slit, for example, blocks red and blue but passes yellow and green. The second monochromator is designed for spectral recombination. The yellow and green rays that enter the intermediate slit at different positions and angles are recombined into a beam that is spectrally homogenous across the exit. The second monochromator has no influence on the spectral transmission. The entrance and intermediate slits determine the bandpass. The exit slit is almost superfluous; yet the light emerging from the exit has a very useful uniformity.

Homogenous Excitation Energy

One of the earliest applications of subtractive dispersion was in the excitation side of spectrofluorimeters. In a typical spectrofluorometer, light from an arc lamp is filtered by a monochromator and directed to a sample cuvette (Figure 2). This narrow bandwidth energy induces fluorescence at different wavelengths. A monochromator/detector combination looks at this emitted fluorescence. If the excitation section of the fluorometer uses an ordinary monochromator, then the illumination of the cuvette will vary spectrally with the position of the cuvette.

Subtractive dispersion homogenizes the beam so that each area in the cuvette sees the same spectral excitation, resulting in increased accuracy. Similar considerations apply to both the detection half of fluorometers and to spectrophotometers. In both, subtractive dispersion has been used to make spectral transmission independent of physical position.

A bonus in the use of subtractive dispersion in fluorometry is reduction of stray light. Stray light in a monochromator originates primarily in scattering at the surface of the grating. Not only is the diffracted light of the desired wavelength directed to the exit slit, but also light that is scattered from scratches, pits, dust and imperfections from the ruling process. The second monochromator acts as a filter for this scattered light reducing it by almost the square of the ratio for a single instrument.
Timed Resolved Laser Spectrometry

The advent of time-resolved laser spectroscopy in the sub-nanosecond regime has created a new application for subtractive dispersive instruments. A conventional single monochromator introduces not only spectral dispersion, but temporal dispersion as well. The temporal dispersion originates in the unequal optical path lengths in the diffraction from the grating.

In Figure 3, the plane wave AB strikes the grating and the diffracted wave is CD. The path of the light that is diffracted from the left edge of the grating, ALC, is longer than the path of the light that strikes the right edge of the grating, BRD. The path difference, $W \times \sin \theta$, gives a temporal dispersion of $W \times \sin \theta / c$. With a typical 68mm wide grating used near 30 degrees, a temporal broadening of 100 picoseconds is the result. A subtractive dispersion instrument removes this instrumentally induced temporal dispersion. The second monochromator introduces an equal and opposite delay across the face of its grating. The degree of cancellation is only limited by the optical aberrations of the systems. In the DK242 and CM112, sub-picosecond residual broadening results.

Monochromatic Imaging

Monochromatic imaging can also benefit from subtractive dispersion. Imaging objects at monochromatic wavelengths has grown from its roots in the Lyman-alpha mappings of the sun. Fluorescent imaging of biological materials now permits direct measurements of positively charged ion concentrations in living cells. Combustion analysis also relies upon optical mapping. In many cases this mapping is being done with filters because of the image smear introduced by a conventional monochromator. Imaging through monochromators uses one of two methods: the object is imaged near the entrance slit, or the object is imaged on the grating (at infinity). In the first method, different wavelength images overlap at the exit slit. In the second method, the monochromatic images that are passed by the monochromator exit at wavelength dependent angles.

The subtractive dispersion instrument cancels both effects, making either form of monochromatic imaging possible. Unlike the conventional monochromator, the subtractive dispersion instrument offers a one-to-one wavelength-independent correspondence between the positions and angles of rays at the exit and entrance.
The Digikrom double monochromators employ a single intermediate slit, housing the two optical paths in one integral unit. This maintains the integrity of the stray light and imaging capabilities while offering ease of use and compactness. As you can see, subtractive dispersion is becoming a more commonly used technique today. Keep it in mind, whether your application is fluorescence, spectrophotometry, time-resolved spectroscopy or monochromatic imaging.

**Digikrom and Spectram Slits - Adjustable and Fixed**

Fixed-interchangeable slits are available on all SP eighth-meter monochromators and spectrometers. Computer controlled variable slits are standard on quarter-meter and larger monochromators and spectrographs. In both cases the slit jaws are thin, typically 25 microns, to reduce tunneling. The materials selected are durable, typically stainless steel, molybdenum, or beryllium-copper. The fixed slits are precisely manufactured so that the width and jaw parallelism is exact to within 5 microns for wide slits and 2 microns for slits with a width of less than 50 microns. The adjustable slits are interferometrically adjusted at SP to better than 2 micron parallelism and width accuracy.

Separation of the slit jaws must be precisely known so that the bandwidth will be exactly known. The slit jaws must be parallel so that the bandwidth for light will be the same at the top and bottom of the slit. The entrance and exit slits must be parallel because the entrance slit is imaged onto the exit slit as the grating is rotated. The slit jaws should be thin compared to their separation, so that tunneling does not reduce the acceptance angle of incident light.

The adjustable slits are computer controlled. A stepping motor and precision lead screws are used to change the separation of the slit jaws thereby adjusting the slit width and the monochromator bandpass. When power is first applied to the instrument, the slit jaws automatically self-calibrate then assume a 50 micron separation. The user from a controller or computer may then program slit width and therefore bandwidth.

**Array Spectrometers - Multi-channel Detection with Improved Signal-to-noise**

In recent years the combination of array detector and spectrograph has become the system of choice for spectroscopy. The major advantage of the array detector is improvement in detection signal-to-noise (S/N) ratio.

An array of N elements has the capability of collecting N times the signal of a single detector. Observation of N units of time with a spectrograph allows a potential improvement in S/N to N^{1/2} opposed to a single detector sampling for one unit of time. Alternatively, N wavelength bands can be sampled in just 1/N the time required for a single detector to do sequentially for identical S/N. This is termed the Fellgate advantage.
In practice the improvement in S/N may be reduced due to the following reasons:

1) Currently available array elements have limited heights, for example 1 to 2 millimeters at most as opposed to 10 to 20 millimeters for a non-array detector.

2) Frequently, only 20% of the array elements have an interesting signal.

3) The switching noise associated with the multiplexed readout of some arrays will frequently double the noise level.

4) When the array element width is smaller than the desired bandwidth, several elements must be combined.

Combining the above effects implies a reduction in the estimated improvement by a factor of 10 to 300. Therefore, for an array with small number of elements, this improvement becomes insignificant.

Array detection has some other advantages. Very rapid multiple wavelength sampling is possible. Moving parts as in a scanning monochromator are eliminated.

SP provides the Digikrom line of high performance spectrographs and a wide selection of CCD and InGaAs cameras covering spectral ranges from UV to NIR. Our SpectraM product line suits your need for a compact, low cost and high performance CCD spectrometer.

**Anastigmatic Imaging - Keeping the Images Sharp**

Spectrometers, like other optical instruments, exhibit aberrations. Coma, spherical aberration and astigmatism are usually the worst offenders to a spectrometer performance. A spectrometer such as a Czerny-Turner spectrometer employs a diffraction grating together with collimating and focusing mirrors. Any aberration introduced by the mirrors will be transformed by diffraction to the exit focal plane. Using appropriate design parameters can compensate coma in a Czerny-Turner spectrometer. Astigmatism causes a point at the entrance slit to extend tangentially at the exit after image transfer, see Figure 4(a). This extension is primarily attributed to the higher order aberrations associated with the use of spherical mirrors. In a spectrograph application a two-dimensional detector array is usually employed at the exit focal plane of a spectrometer. The astigmatism can thus cause a serious energy spread, limiting the multi-channel spectrometer to a device for virtually single input at the entrance. SP Digikrom series spectrographs offer astigmatism corrected options. The use of specially designed aspherical optics corrects for astigmatism in the wavefront produced by spherical mirrors, Figure 4(b). The anastigmatic optics in turn result in highly energy concentrated images at the exit and tightly focused spots. Multiple inputs along the entrance slit are thus made possible with SP anastigmatic spectrographs.

Figure 5(a) demonstrates a multiple spectral input Raman application by use of a SP spectrograph equipped with a two-dimensional CCD camera. Four fiber inputs are presented at the entrance as shown in Figure 5(b). SP anastigmatic spectrographs allow for inexpensive versatile and multi-functional spectroscopic applications.
Miniature Spectrometers - Compact, Stable, Sensitive, Unique and Low Cost

SP SpectraM miniature spectrometers are packed with great features and performance in a small footprint. The SM series spectrometers are based on a crossed Czerny-Turner configuration as shown in Figure 6. A light input through the slit, either fiber coupled or direct coupling is collimated by the first mirror and directed to a diffraction grating. The diffracted light is collected by the camera mirror and focused onto a detector array for detection. The spectrograph is enclosed in a rugged aluminum housing for stability. Connections between the spectrometer and the computer interface are made via a shielded electrical cable. Detector arrays are also included in the same housing in hand held versions. SM spectrometers can be interfaced to computers via ISA, PCI, PCMCIA, etcetera. By use of a PCMCIA interface with a notebook computer, Figure 7, the SM spectrometers place a powerful portable spectrometer system at your fingertips.

It is known that all detectors exhibit “dark signals” originated from thermally agitated electrons. A temperature increase of 7°C can result in a doubled dark signal in a silicon-based detector. SP offers cooled SM spectrometers for greater temperature stability for demanding applications. Uncooled SM spectrometers are also available for low cost detection use. The separation of the spectrometer module from a heat source such as a computer ensures reasonable temperature stability.

SM spectrometers employ detector arrays with high sensitivity. A sensing element height of 200mm to 2.5mm maximizes the detector light collection capability. A cylindrical focusing lens in front of the detector array further enhances the effective pixel size. In addition, for UV and near IR regions where silicon detector response is inherently weak, we provide a variety of sensitivity enhancement coatings for detector arrays. Our pioneering optics and coating technologies also allow us to take another step further to reduce energy lost between optical surfaces.

As discussed before, all gratings generate higher orders. By use of SP’s unique variable filters in SM spectrometers, a wide simultaneous wavelength coverage is achieved free of higher order interferences. Our continuous product development effort is adding to the uniqueness of our spectrometer line everyday. For example the compact double Czerny-Turner spectrometer from SP, which needs only one detector array, is the first in the world.
Issues with Using Lasers as Light Sources with Spectrometers

1. Underfilling the grating. The resolution of a monochromator is limited by the number of grating grooves that are illuminated. Written mathematically:

\[ R = \frac{m}{N} \]

As an example, an unexpanded HeNe laser with a beam diameter of about 0.3mm used directly on a 1200 groove-per-millimeter grating in a monochromator will have a best resolution of:

\[ \frac{633.2 \text{ [nm]}}{1200 \times 0.3} = 0.8\text{[nanometer]} \]

Expanding a 0.3mm laser beam to fill a 68mm grating can be difficult. One of the simplest ways is to place a diffuser near the slit or use an integrating sphere, and illuminate that diffuser with a moderately expanded beam. For an f/4 monochromator with a diffuser 4 millimeters from the slit, the beam spot on the diffuser needs to be only a 1 millimeter diameter.

2. Melting the slits. The slits of monochromators are typically stainless steel that tapers to a 0.001" thickness at the tip. Experience with pinholes has shown that even a few hundred milliwatts (CW) or a fraction of a Joule (Pulsed) will melt 0.001" thick stainless steel.

The best solution is to use a beamsplitter to send only a small fraction of the beam to the monochromator. The 0.3% reflection from an antireflection coated plate is usually more than sufficient for measurement.

Another solution is to not use the slit. The laser beam, focussed at the slit plane, will act as its own slit. Be warned, however, that the laser beam will be refocussed by the monochromator at the exit slit. That exit slit then is in danger of melting.

3. Melting the grating. Grating surfaces are typically micron thick aluminum that is bonded to the glass substrate by a thin epoxy resin; the aluminum will have about 6% absorption. At high CW powers (about 20kW/cm²) the thermal heating due to the absorption will cause the epoxy to melt. At high pulsed power (about 2 MW/cm²) the aluminum will ablate. In either case the grating is destroyed.

The solutions are the same as given in cases One and Two above. The power input into the monochromator can be attenuated. The beam can be expanded to use the whole grating area. Note that the area of a 68mm grating, 46 cm², is sufficient for pulse powers of about 0.1 GW.
Maximizing performance for SP Instrumentation

SP spectrometers are designed to meet the highest performance standards. To ensure the designed performance is achieved, it is also important that the instruments are set up and optimized.

1. When coupling light into and out of a spectrometer, f# matching is helpful for efficient coupling. f# matching helps to minimize stray light introduced by overfilling the spectrometer optics. In many instances, a simple aperture behind the coupling optics works efficiently for this purpose. Figure 8 depicts a spectrometer light coupling system which uses f# matching optics together with a mechanical aperture.

2. Incident radiation into a spectrometer with a band broader than necessary may have a negative impact on the instrument’s stray light performance. A tungsten halogen lamp, for example, emits radiation from about 320nm to over 2000nm. In applications where only the visible spectrum, 400 to 700nm, is concerned the use of a band pass filter can minimize the stray light arising from dumping the entire band into a spectrometer. Measurement signal to noise ratio can thus be improved.

3. All grating instruments exhibit higher diffraction orders originating from the use of diffraction gratings (see also Spectrometer Basics section). Ignoring the higher orders, especially the second order contribution may result in serious errors. Use of SP filters or filter wheels may remove the second order. The optimum position for the placement of such a filter is in front of the instrument entrance whenever possible.

4. Filter wheels are not limited to order sorting purposes. SP’s automatic filter wheels are ideal for use in variable ratio beam splitting, variable beam attenuation and other applications when mounted with appropriate optics.

5. Fibers operate based on total internal reflections, Figure 9. Light transmitting characteristics for fibers may change with bending curvature and positioning of coupling. When fiber input is selected for SP spectrometers it is a good practice to minimize the change in fiber bending curvature during operation. Fibers with precision positioning couplers, such as offered by SP, are highly recommended for repeatability and maximum light coupling.

6. When using scanning monochromators be aware that resolution will be lost if data is not collected at sufficiently fine wavelength increments. In a continuous scan mode the maximum scan rate at which the instrument resolution will be maintained is also dictated by the Nyquist theorem. Instrument resolution will degrade with an increase in scan speed exceeding the Nyquist limit.
7. Gratings and other optical components are delicate and precise optics. Any attempt to clean them with inappropriate methods may cause scratches and other damage, leading to performance degradation.

8. The relationship between the slit widths and bandpasses can be calculated by multiplication of reciprocal dispersion with the slit width. For example, a monochromator configured with 0.25 millimeter slits and a grating displaying a reciprocal dispersion of 8 nm/mm has a bandpass of 8 * 0.25 = 2nm.

9. In array detection on a spectrograph such as a CCD camera mounted onto the DKSP240 spectrograph or a SM240 spectrometer, the minimum resolution element is three array elements (pixels). As pixels are typically 14 microns wide, the effective slit width is 42 microns in this case. This would equate to 0.3 nanometers on a 1/8 meter spectrograph utilizing a 1200 g/mm grating.

Applications with SP Instruments

SP instrument products have found wide applications in many areas for light illumination, light detection and other usage. It is beyond the scope of this catalog to attempt to cover all these aspects. However for the benefit to our customers, we demonstrate here some general application configurations.

Figure 10 illustrates a tunable light source, which consists of a wide band light source and a SP scanning monochromator. The output wavelength can be programmed for continuous scan or a selected narrow band.

Figure 11 (next page) shows the above tunable light source equipped with a bifurcated fiber for a dual beam type of arrangement. One of the fibers can be used to couple the narrow band light to a sample channel for transmittance, reflectance, absorption or other measurement use. The second fiber directly introduces a portion of the narrow band output from the monochromator into a reference detection channel. Using the reference channel can compensate any possible fluctuation in the output light intensity in the measurement channel, since they are all derived from the same source. In this sense a so-called “dual beam” or “double beam” system can be established. With SP fiber couplers, light can be introduced in and out of SP spectrometers for flexibility and remote capability.

On the next pages, Figures 12 through Figures 18 review some typical application arrangements with SP SM spectrometers for transmittance, reflectance, absorption and emission measurements.

SP’s monochromators and spectrographs have features that are unduplicated in any other spectrometers. For this reason, they have been applied in unique applications. The following are a few examples.
Figure 11. Diagram for a dual-beam illumination source by use of a SP monochromator.

Figure 12. Direct transmittance/absorbance measurement with SM spectrometers.

Figure 13. Transmittance/absorbance measurement by use of a fiber optic immersive probe.

Figure 14. Transmittance/absorbance measurement with SM spectrometers via optical fibers.

Figure 15. Reflectance measurement with SM spectrometers by use of 45° configuration via optical fibers.
Figure 16. Direct reflectance measurement performed with a 45° attachment and an SM 240 spectrometer.

Figure 17. Dual-beam transmittance/absorbance setup involving two SM240 spectrometers connected via fibers.

Figure 18. Dual-beam 45° reflectance measurement by use of two SM240 spectrometers via fiber connection.
Constant Energy or Bandpass Spectrophotometry

The slits in SP’s larger monochromators are computer controlled. Usually, the slits are set for a particular width. However, when the monochromator is used in a spectrophotometer it is possible to adjust the slits to maintain constant energy or constant bandpass.

The spectrophotometer consists of a lamp, the monochromator, a sample, and a detector. The overall system response is not flat over the entire spectral range. By adjusting the slit width at each wavelength increment during a scan, constant signal size can be maintained. The same settings can then be used for reference or sample measurements.

In the above adjustment fashion the actual spectrometer bandpass is varied with the slit width since the grating dispersion changes with the wavelength. In applications where constant bandpass is necessary, the slit width on SP monochromators can be adjusted via computer control.

Dual Excitation Microfluorescence

The compact size and low price of SP’s 1/8 meter monochromators enables them to be used in place of filters. The simple, internal computer interface allows these monochromators to be much more than a fixed filter replacement.

For example, in a dual-excitation micro-fluorescence system, two xenon arc lamps direct light into two SP 1/8 meter monochromators. The exits are coupled through fast shutters into two halves of a bifurcated fiber bundle. The exit of the bundle provides fast, tunable, dual-wavelength, epifluorescent illumination for a Zeiss microscope. By using SP’s 1/8 meter monochromator, the system has been made compact and computer controlled.

Time Domain Spectroscopy

Pulsed laser fluorescence spectroscopy is increasingly interesting because of the extra information that the time domain provides. However, if a conventional monochromator is used to clean up the excitation beam or analyze the emission, the monochromator will broaden the pulse by several hundred picoseconds.

Porta Radiometry

Field measurements of lamps, reflection and transmission require more range, accuracy and computer compatibility than a commercial colorimeter will provide. With SP’s 1/8 meter monochromator and AD130 smart detector, or an SM spectrometer and a notebook computer, a research grade radiometer can be slipped into a briefcase. The briefcase would still have room for standards, notes, and perhaps an AF series fiber optic probe and interface to make sampling easy. Both approaches make a complete computer compatible system in a very small package.

Detection Systems for Tunable Lasers

Tunable lasers such as Ti:sapphire and optical parametric lasers are finding more applications as excitation sources in laser spectroscopy. SP scanning monochromators and array spectrometers are capable of synchronized detection in such experiments. In one application a Digikrom monochromator was programmed to follow the wavelength scan of an OPO laser for detecting fluorescence. In another setup with a Ti:sapphire laser tuning through a spectral range, an SM spectrometer was used to monitor the laser radiation wavelength in a real time mode.
A Guide to Spectrometer Selection

The choice of a spectrometer must be guided by the application requirements. The parameters that delineate most applications are listed below:

1. Is the needed output a single wavelength or a dispersed spectrum? Monochromators select single wavelengths, spectrographs have dispersed spectral outputs.

2. Is high resolution (high dispersion) or low resolution (low dispersion) needed? The greater the resolution that is needed, the longer the focal length of the monochromator should be. A spectrograph with greater resolution will necessarily have a smaller bandpass. High resolution also dictates a narrow slit width in array spectrometers.

3. Does the spectrometer need to select a weak signal in a strong light background? If stray light rejection is important, then a double monochromator may be necessary.

### Table 1. Selection Chart by Applications

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<tr>
<th>Application</th>
<th>Requirements</th>
<th>Recommended</th>
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<tbody>
<tr>
<td>Fluorescence</td>
<td></td>
<td></td>
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<tr>
<td>Fluorescence in liquids (emission or excitation)</td>
<td>1-20nm bandwidth Good stray light rejection</td>
<td>CM110 1/8 meter monochromator or SM spectrometer for emission detection</td>
</tr>
<tr>
<td>Fluorescence in biological materials (emission or excitation)</td>
<td>1-20nm bandwidth Excellent scattered light rejection</td>
<td>CM112 1/8 meter monochromator or SM spectrometer with special filter</td>
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<tr>
<td>Fluorescence in solids (emission or excitation)</td>
<td>0.2-3.0nm bandwidth Good stray light rejection</td>
<td>DK240 1/4 meter monochromator or SM GT2 spectrometer for detection</td>
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<tr>
<td>Weak fluorescence in solids, liquids (emission)</td>
<td>Array detection for high sensitivity 0.2-3.0nm bandwidth</td>
<td>DKSP240 1/4 meter spectrograph with array detection system</td>
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<tr>
<td>Weak fluorescence in scattering biomaterials (emission or excitation)</td>
<td>High stray light rejection High sensitivity</td>
<td>DK240 1/4 meter monochromator</td>
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<tr>
<td>Phosphorescence, fluorescence kinetics (emission)</td>
<td>Array detection for time resolution</td>
<td>DKSP240 1/4 meter spectrograph with array detection system</td>
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**continued**
### Table 1. (continued) Selection Chart by Applications

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<th>Application</th>
<th>Requirements</th>
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<td>Spectrophotometry</td>
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<tr>
<td>Spectrophotometry of clear liquids, optics</td>
<td>1-20nm bandwidths to 0.1% transmission</td>
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<td>Spectrophotometry of gases, traces in clear solids</td>
<td>To 0.01% transmission 0.05-1.0nm bandwidth</td>
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<td>Spectrophotometry of dense objects</td>
<td>To 0.001% transmission, 1-20nm bandwidths. High sensitivity</td>
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<td>Time varying spectrophotometry (thin film monitoring)</td>
<td>Array detection</td>
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#### Laser Spectrometry

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<td>Picosecond studies liquids, biological materials</td>
<td>Preserving pulse width 1-20nm bandwidths</td>
<td>CM110, CM112 monochromators</td>
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<tr>
<td>Picosecond studies solids, gases</td>
<td>Preserving pulse width 0.2-2.0nm bandwidths</td>
<td>DK240 1/4 meter monochromator</td>
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<tr>
<td>Tuning, wavelength checking, diode lasers</td>
<td>Resolution, accuracy to 1.0nm</td>
<td>CM110 1/8 meter monochromator</td>
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<tr>
<td>Tuning, wavelength checking, gas and dye lasers</td>
<td>Resolution, accuracy to 0.1nm</td>
<td>DK140 1/4 meter monochromator</td>
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<tr>
<td>Diode laser mode structure</td>
<td>Resolution to 1.0nm</td>
<td>CM110 1/8 meter monochromator</td>
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#### Emission Spectrometry, Radiometry

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<th>Requirements</th>
<th>Recommended</th>
</tr>
</thead>
<tbody>
<tr>
<td>Arc, spark, or plasma spectroscopy</td>
<td>Resolution to 0.03nm</td>
<td>DK480 1/2 meter monochromator</td>
</tr>
<tr>
<td>Arc, spark, or plasma spectroscopy of small traces</td>
<td>Resolution to 0.03nm array capability</td>
<td>DK480 1/2 meter monochromator and spectrograph</td>
</tr>
<tr>
<td>LEDs, incandescent lamps, fluorescent lamps, phosphors</td>
<td>1-20nm bandwidth</td>
<td>CM110 1/8 meter monochromator or SM spectrometer</td>
</tr>
<tr>
<td>Raman spectrometry</td>
<td>0.3-10 cm(^{-1}) bandwidth Excellent stray light rejection</td>
<td>CM110 1/8 meter monochromator with special filter, CM112 double monochromator</td>
</tr>
</tbody>
</table>
Notes

Biological samples frequently scatter almost 100% of the incident light. To detect a weak fluorescence signal in this environment requires a double monochromator, frequently on both the excitation and emission sides.

Array detection can potentially multiply the signal collected by the number of detector elements, N. The signal to noise ratio potentially improves by the square root of N.

Plane and Holographic Gratings

In recent years spectrometers using corrected concave holographic gratings have been heavily promoted. The advantages of these instruments are compactness, few optical elements and aberration correction that improve resolution.

Why has the plane-grating spectrometer survived? For the UV, for the IR, for wide spectral ranges, and for radiometry in which absolute intensity of a signal is important, the plane-grating spectrometer is superior.

Corrected concave-gratings offer good resolution over a wavelength octave, typically 350nm to 700nm. Outside of this region, the aberrations are much worse than those in a plane-grating instrument are. A typical Czerny-Turner monochromator with a 1200 groove-per-millimeter plane grating will have a good resolution from 250nm to 1500nm, over three times the wavelength range of its concave grating counterpart. The plane-grating spectrometer offers superior resolution in the UV and IR.

Concave-grating instrument designs are generally good for one spectral region only. Changing gratings is not possible. Plane-grating spectrometers can change their spectral region by changing gratings. A Czerny-Turner spectrometer with a triple grating turret can span 200 to 2000nm with good resolution and good efficiency.

Table 1. (continued) Selection Chart by Applications

<table>
<thead>
<tr>
<th>Application</th>
<th>Requirements</th>
<th>Recommended</th>
</tr>
</thead>
<tbody>
<tr>
<td>Infrared Spectrometry</td>
<td>1-20nm bandwidth 200-2500nm tunability</td>
<td>CM110, DK240 monochromators or multiple SM spectrometers</td>
</tr>
<tr>
<td>Fiber analysis, LED analysis source or detector</td>
<td>1-20nm bandwidth 700-1100nm tunability</td>
<td>CM110, DK240 monochromators or SM spectrometers</td>
</tr>
<tr>
<td>NIR spectrophotometry</td>
<td>1-20nm bandwidth 700-1100nm tunability</td>
<td>CM110, DK240 monochromators or SM spectrometers</td>
</tr>
<tr>
<td>General Purpose</td>
<td>Array capability 200-20000nm tunability 0.3-30nm bandwidth</td>
<td>CM110, DK240 monochromators and spectrographs or SM spectrometers</td>
</tr>
<tr>
<td>Teaching, general lab use</td>
<td>Array capability 200-20000nm tunability 0.3-30nm bandwidth</td>
<td>CM110, DK240 monochromators and spectrographs or SM spectrometers</td>
</tr>
</tbody>
</table>
Concave-grating spectrometers have transmission efficiencies that vary greatly with the input angle. This makes them poor choices for radiometric studies in which the intensity at each wavelength is critical and uniform illumination of the grating cannot be guaranteed. Because the groove profiles of corrected concave gratings vary greatly across the grating surface, the diffraction efficiency also varies greatly across the surface. This contrasts with the plane-grating which has the same efficiency at all points on the surface. Unless the light enters a concave-grating instrument in exactly the same distribution each time, the instrument will have varying transmission efficiency. Fifty-percent changes from central illumination to edge illumination have been measured.

Corrected concave-gratings average half the diffraction efficiencies of plane-gratings. The groove profile of a ruled-plane grating is designed for high efficiency within narrow limits. Ion etching has been used to sharpen the groove profiles of corrected concave-gratings, but this is akin to making a lens from a glass plate by sandblasting. The profile improves, but the surface and scatter are horrible.

While corrected-concave-grating spectrometers occupy an important niche in spectroscopy, plane-grating instruments remain the workhorses.

Gratings and Their Selections

From the foregoing discussion on grating equation it is clear that the longest wavelength that will be diffracted by a grating is 2*d. This places a long wavelength limit on the spectral range of a grating. The table below illustrates this limit. Loss of light as the grating is rotated to a steep angle usually limits the actual range to about 90% of the long wavelength limit listed.

The wavelength dependence of grating efficiency also constrains the spectral range. SP has a complete set of diffraction efficiency curves for all of its standard and custom gratings, and the appropriate curves should be reviewed if spectral range is important.

Table 2. Grating Density and Long Wavelength Limit

<table>
<thead>
<tr>
<th>Grating Density (g/mm)</th>
<th>Groove spacing (nm)</th>
<th>Long-wavelength Limit (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>3600</td>
<td>277.78</td>
<td>555.56</td>
</tr>
<tr>
<td>2400</td>
<td>416.67</td>
<td>833.33</td>
</tr>
<tr>
<td>1800</td>
<td>555.56</td>
<td>1,111.11</td>
</tr>
<tr>
<td>1200</td>
<td>833.33</td>
<td>1,666.67</td>
</tr>
<tr>
<td>600</td>
<td>1,666.67</td>
<td>3,333.33</td>
</tr>
<tr>
<td>300</td>
<td>3,333.33</td>
<td>6,666.67</td>
</tr>
<tr>
<td>150</td>
<td>6,666.67</td>
<td>13,333.33</td>
</tr>
<tr>
<td>75</td>
<td>13,333.33</td>
<td>26,666.66</td>
</tr>
<tr>
<td>50</td>
<td>20,000.00</td>
<td>40,000.00</td>
</tr>
</tbody>
</table>
Selection by Required Bandwidth or Dispersion

A table giving typical reciprocal linear dispersions near the center of the spectral range is given below.

The bandwidth transmitted by a monochromator will be the dispersion times the slit width. Given two of the three variables-bandpass, slit width and dispersion-the third can be calculated.

Most applications are light starved, and it is useful to open the slits to the greatest width that is compatible with the desired bandwidth. To increase the slit width while retaining the bandwidth, one can select a higher groove density. For example, at 340nm and a 10nm bandwidth in a 1/8 meter monochromator, a 1200 g/mm grating will allow a 1.4nm slit width, but a 2400 g/mm grating will allow a 2.8 millimeter slit width at the same bandpass.

Occasionally, the bandwidth may be constrained by the maximum slit width. A typical 1/4 meter monochromator might have a maximum slit width of four millimeters; a 14 nanometer bandpass would result with a 1200 g/mm grating. If a 28nm bandwidth was desired, a 600 g/mm grating would give the required bandpass.

For spectrographs, a particular dispersion is frequently desired. To cover 400 to 700 nanometers on a 25mm array detector would require a dispersion of 12nm/mm. The grating suitable for this dispersion for an SM2XX spectrometer would be a 1200 g/mm.

A particular resolution might also be required in a spectrograph. To resolve 0.3 angstroms in three pixels (75 microns) would require a dispersion of:

\[
\text{\( \frac{0.03}{0.075} \) = 1.3nm/mm.}
\]

This dispersion would be typical of an 1800 g/mm grating in a 1/2 meter spectrograph.
Selection by Required Throughput

One frequently needs to obtain the maximum grating efficiency for a particular wavelength band. It would be useful to be able to design a groove profile to provide that efficiency profile. Unfortunately, this problem has not yet been solved. In practice, the efficiencies of many gratings have been measured; one selects from the grating with the desired efficiency curve.

For ruled gratings and blazed holographic gratings the efficiency profile is generally triangular. The grating is most efficient at a blaze wavelength, $\lambda_b$. While a number of blaze wavelengths are generally available, the most common is $1/3$ of the long wavelength limit. (For a 1200g/mm grating, this would be at 500 nanometers.) The peak at $\lambda_b$ usually 90%, and the efficiency falls to about 20% at $0.67 \times \lambda_b$ and at $1.5 \times \lambda_b$.

Holographic gratings generally have flat efficiency profiles. The mean efficiency is about 30% over a range of $0.33 \times \lambda_b$ to $1.5 \times \lambda_b$. In both cases, real efficiencies show complicated polarization dependence. The ratio of efficiency for polarization parallel to the groove to that perpendicular to the grooves may be 3:1 over a large spectral range.

In Figure 19, typical efficiency curves for a standard SP grating are presented. These curves span a wide range of wavelengths from UV to IR. These curves do not account for loss of solid angle of the grating as it is rotated. In addition to the curves included here, SP has measured efficiencies for both polarized and unpolarized light on a wide variety of other gratings; this data is available upon request.

Selection by Stray Light Level

Both scatter and extraneous spectral features (ghosts) may result from grating imperfections (see Stray Light discussion in Spectrometer Basics section). These imperfections result from the grating manufacturing processes. In general there are five types of gratings available; interferometrically ruled, ruled, holographic, sheridan blazed holographic and ion-etched holographic.

Interferometrically ruled gratings, holographic gratings and sheridan blazed gratings have comparable levels of stray light. All three are generally free of ghosts. Exposing photoresist with a laser generated interference pattern makes the holographic gratings. The interference pattern is sinusoidal so the resulting groove shape is sinusoidal. These gratings generally have low efficiency. Sheridan blazed gratings are produced by exposing the photoresist from both sides. A triangular profile results; these gratings have good efficiency. However, the technique will only produce UV blazed gratings. In ruling gratings, a pointed diamond is used to burnish the groove profile into a gold film on a quartz substrate. The position of the diamond is controlled by an interferometer as each groove is cut.

Classical ruled gratings are ruled without interferometric control. These gratings tend to have small, periodic errors in their groove profile.

SP's standard gratings are listed in Appendix A. Standard DK24 series gratings are 68mm x 68mm. Wide gratings (64mm x 84mm) are available. SP's standard DK12 series gratings are 30mm x 30mm. For gratings not listed consult SP.

Recommended applications are listed next page for ruled diffraction gratings using spectral range, bandwidth, throughput and stray light selection criteria discussed above.
# Selection by Application

## Table 4. Selection of Gratings by Applications

<table>
<thead>
<tr>
<th>Application</th>
<th>Grating g/mm</th>
<th>Grating Blaze Wavelength (nm)</th>
<th>DK</th>
<th>CM</th>
<th>SM</th>
<th>Remarks</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fluorescent illumination</td>
<td>2400</td>
<td>240</td>
<td>X</td>
<td>X</td>
<td></td>
<td>Highest UV through-put</td>
</tr>
<tr>
<td>Fluorescent detection</td>
<td>1200</td>
<td>500</td>
<td>X</td>
<td>X</td>
<td></td>
<td>Efficient over emission range</td>
</tr>
<tr>
<td>NIR laser analysis</td>
<td>600</td>
<td>1000</td>
<td>X</td>
<td>X</td>
<td></td>
<td>Efficient over emission range</td>
</tr>
<tr>
<td>NIR laser analysis</td>
<td>1200</td>
<td>1000</td>
<td></td>
<td></td>
<td>X</td>
<td>Efficient over emission range</td>
</tr>
<tr>
<td>Raman</td>
<td>1800</td>
<td>500 holographic</td>
<td>X</td>
<td>X</td>
<td></td>
<td>Fair efficiency, good stray light performance</td>
</tr>
<tr>
<td>NIR Raman</td>
<td>600</td>
<td>1100</td>
<td>X</td>
<td>X</td>
<td></td>
<td>Good efficiency, good stray light performance</td>
</tr>
<tr>
<td>UV-VIS Array</td>
<td>300</td>
<td>300</td>
<td>X</td>
<td>X</td>
<td></td>
<td>Good efficiency, covers UV and part of visible</td>
</tr>
<tr>
<td>UV-VIS Array</td>
<td>1200</td>
<td>250</td>
<td></td>
<td></td>
<td>X</td>
<td>Good efficiency, covers UV and part of visible</td>
</tr>
<tr>
<td>VIS Array</td>
<td>300</td>
<td>500</td>
<td>X</td>
<td>X</td>
<td></td>
<td>Good efficiency, covers entire visible region</td>
</tr>
<tr>
<td>VIS Array</td>
<td>600-1200</td>
<td>550</td>
<td></td>
<td></td>
<td>X</td>
<td>Good efficiency, covers entire visible region</td>
</tr>
</tbody>
</table>