What's the Right Spectrometer for You?

Whether you are a research scientist or an OEM integrator, Ocean Optics appreciates that selecting a spectrometer, optical sub-system or complete spectroscopic solution is a critical decision. We see ourselves as your partner in that process. We work to understand your application, your customers and your business model. As a true business partner, we:

- provide technology leadership
- protect your investment through custom development and sustaining engineering
- help you manage costs by constantly improving our manufacturing efficiencies

A key element of our partnership with all our customers is the sharing of our knowledge and application expertise. In this whitepaper, we cover some of the fundamental technical issues to consider in selecting a spectrometer for your optical sensing application.

Choosing a spectrometer for your new product is similar to choosing a spectrometer for your lab experiment. However, there are additional considerations that relate to making a product tailored to your application requirements, to the growing scale of your business and to the specific needs of your customers.

Understanding the Application Landscape and Your Customer’s Needs

Our partnership process starts with understanding the big picture of your business model and its focus on the customer, and drills down into the specific product needs to deliver a complete solution. While the need to balance price and performance is obvious, what is not always clear to OEM and academic customers is the importance of linking the spectrometer to the application. While ultimately this is distilled into a product specification, the route to that specification begins at the sample and the measurement application.

Advances in optical and spectroscopy technology make measurements that were once performed by very sophisticated laboratory instruments accessible to everyone. Specifically, miniature spectrometers make a world that once required returning the sample to the laboratory obsolete. Now, spectroscopy can be carried out near the sample: in the manufacturing process, beside a patient’s hospital bed or inside an erupting volcano. Liberating the measurement from the laboratory takes optical sensing to the next level -- unlocking numerous applications and creating new and expanding markets.

The ability to customize a miniature spectrometer enables systems that solve specific application problems. Whether measuring absorbance, reflectance or the Raman peaks, these tools give information that deliver a targeted answer. In order to deliver a properly specified component or system, the information that the optical system will deliver and the problem that your product helps the customer overcome must be well understood. A complete understanding of the measurement application throughout the process drives to the proper final product specifications.

Lastly, the product you produce must meet or exceed customer expectations. This is not purely a question of addressing a level of technical competence; it also includes the overall customer experience and the proper fit of the product into the customer’s workflow. From the viewpoint of the OEM, this means complete understanding of the product’s form, fit and function. The risk of poor market reception can be mitigated by having a comprehensive understanding of the product’s critical performance needs and keeping these requirements top of mind through the development process.
Developing and Configuring a Solution

The selection of a spectrometer involves a series of trade-offs among different optical parameters. In order to understand these trade-offs we must first understand the components of the optical bench and their role in segregating and measuring the spectrum. A typical cross Czerny-Turner spectrometer is shown in Figure 1. The optical bench comprises an entrance slit (1), a folding mirror (2), the grating (3), a focusing mirror (4) and the detector (5). The entrance slit, grating and detector combine to determine the wavelength range and resolution of the spectrometer.

Wavelength Range and Resolution

More specifically, the wavelength range and the resolution are influenced by (a) the size of the entrance slit, (b) the groove density of the grating and (c) the number of active elements (pixels) in the array detector. Let’s examine these parameters, starting with the entrance slit. The optical bench transfers an image of the entrance slit onto the detector such that monochromatic light will fall across all the pixels illuminated by the slit image. The optical resolution is directly related to the slit width. For example, in one bench configuration a 100 µm slit will have an optical resolution of 14.0 pixels FWHM (Full Width at Half Maximum). Decreasing the slit width to 50 µm will improve the optical resolution to 7.4 pixels FWHM, but the throughput of light will be reduced by approximately 50%. As the slit width decreases it approaches the limit of diffraction and the improvement in resolution begins to diminish. Moving from a 50 µm slit to a 5 µm slit only improves resolution by a factor of 3.7, instead of the anticipated factor of 10.

Also, the choice of grating and wavelength range must take into account how gratings function. Light striking the grating is diffracted into multiple angles. The angles are whole-number multiples or orders that vary with the incident wavelength, as in Figure 2. For example, incident 200 nm light will be diffracted at angle #1, and at angle #2, which is exactly twice as large as #1. Angle #2 also corresponds to the first order diffraction of light at exactly twice the wavelength, or 400 nm. If the application requires measurements at 400 nm, and 200 nm light enters the spectrometer, light from both the second order diffraction of 200 nm and the first order diffraction from 400 nm will reside at the same pixel. Therefore, the measured intensity at that pixel will include contributions from both wavelengths.

Second order light is removed by using filters. Array spectrometers intrinsically lend themselves to the use of linear variable filters designed to match the dispersed spectra and provide the appropriate blocking at each pixel in an array. Because these linear variable filters are designed and fabricated for a particular bench, grating and starting wavelength, the customer loses the option to adjust the spectral range. Alternatively, light from higher order diffraction can be excluded by filters before entering the spectrometers, preserving the flexibility of the optical bench.

Figure 1: Typical cross Czerny-Turner spectrometer

Figure 2: Dispersion of monochromatic light from the grating illustrating higher order diffraction.
Gratings can be optimized for particular wavelength ranges. This is accomplished by tilting the grooves, called the blaze angle. The efficiency of the first order diffraction is enhanced in one wavelength region, with the trade-off that it decreases in another region. For example, a 600 line/mm grating blazed for optimum efficiency at 300 nm is <30% efficient at wavelengths greater than 575 nm. The same grooves tilted at an angle to accentuate the NIR region are >30% efficient from 530-1100 nm but are low efficiency in the UV. Groove density also influences the available blaze angles. Special composite gratings, like the Ocean Optics HC-1 grating, have regions with different blaze angles. This yields a grating with good efficiency over a wider wavelength range (200-1050 nm) than is possible with traditional gratings.

For example, in our “S” bench, a 600 line/mm grating will cast a 650 nm band of light across the active area of the detector. By rotating the grating, the spectral range illuminating the detector can be varied. This facilitates the measurement of a spectrum from 200-850 nm, or from 300-950 nm, and so on. Substituting a 1200 line/mm grating causes the light to be diffracted at twice the angle, thus the detector will intercept half the wavelength range. Because the same amount of light is spread out over twice the angle the signal will be decreased by a factor of two. With everything else held constant, the optical resolution would be twice as fine.

Physically increasing the size of the optical bench has the net effect of achieving higher resolution at the expense of a narrower wavelength range. The “S” bench is a 42 mm focal length design. The HR bench is a 102 mm focal length design. In the HR bench, the same 600 line/mm grating would yield a range of about 430 nm and resolution that is 66% finer. Of course, the signal is lower because of the higher resolution. The other trade-offs with the longer focal length are size and weight.

Lastly, the choice of detector pixel density drives the optical performance specifications. All other things being equal, the density of the detector elements across the dispersed light determines the resolving power of the spectrometer. If a 1024 element array is replaced with a 2048 element array, the resolution of the spectrometer is improved by a factor of about 2, providing a higher data density over the same operating range. The size of the pixels in the array also imposes a limit on the resolution that can be obtained with a given bench. In general, our detectors have pixel spacing from 8 µm to 14 µm. These detectors are small enough to achieve the maximum resolution possible with our smallest slits.

**Detector Material and Optimization**

Detectors are chosen for several design features. Semiconducting detectors are used to capture photons and convert them into electrons. The absorption band gap of silicon allows for good sensitivity over the ultraviolet (UV), visible and shortwave NIR region (from around 160 nm to nearly 1100 nm). Indium Gallium Arsenide (InGaAs) detectors generally work well above 900 nm to about 1700 nm. Special dopants placed in InGaAs detectors can be used to extend the range from 2100-2500 nm. For example, HgCdTe can extend the measurement range to the mid-IR.

Also, the effective spectral range and resolution for detectors depend on architecture. The simplest design is called a photodiode array (PDA). In PDA detectors, each diode in the array is connected to readout circuitry that occupies a portion of the array next to the detector. The diodes are supplied with a bias voltage, and photons that are absorbed by the Si generate a current. The sampling circuitry features a sample and hold scheme with the ability to strobe through the row of detectors to acquire the voltage signal from each pixel. The stream of analog signals is amplified and converted to digital spectral data by low-noise external circuitry.

The need to produce images, like those in the first photocopiers, fax machines and digital cameras led to the invention of the charge coupled detector or CCD. Here the photodiode is covered by a transparent capacitor that accumulates the signal during a length of time called an integration period. The advantage of this architecture is that there are no dead spots occupied by readout circuitry and images can be captured. A linear CCD array is the same architecture but consists of a single line of CCD devices instead of the bare photodiodes.
CCDs have a great advantage over photodiodes in that they have very low levels of readout noise. Their main disadvantage is that the polysilicon gates or capacitors absorb UV light; CCDs generally do not respond to light much below 350 nm. There are two remedies to this problem. The CCD array can be coated with a phosphor, which absorbs UV light and emits visible light. This renders a detector with adequate UV response for many applications. A more expensive solution is to make the device very thin and to turn it around so it is illuminated from the backside. This exposes the photodiodes to the UV light and the resulting device is significantly more sensitive to UV than the phosphor-coated types.

Some applications require detectors with specific features. For example, time resolved kinetics spectroscopy requires a detector that can be gated. A light source excites the sample at time zero. The detector must be triggered to start collecting the light emitted by the cooling plasma after a microsecond delay. Here it is critical for the detector and therefore, the spectrometer, to communicate externally both with incoming triggers and outgoing data.

**Spectrometer Communication**

We understand that the spectrometer is just one component within your overall system, and it is important to plan how it will communicate with other elements of your system design. For maximum speed, PC communications are generally handled over USB 2.0 when connected to laptops, tablets or embedded computers running Windows, MacOS or Linux. For smaller handheld form-factors, or rigidly deterministic industrial / embedded solutions, we also support RS232, RS422 or lower-level protocols like SPI (EMBED series only).

Besides host-to-spectrometer communications, the spectrometer itself is able to directly time and control secondary peripherals via GPIO (TTL) signaling. These can be used to synchronously pulse strobe lamps, trigger lasers, toggle external shutters, position a linear actuator, or control almost any other accessory which is required by your application. Advanced peripheral control can be achieved through pass-through I2C and SPI pins on most models, providing ultimate flexibility in inner-system control.

All these capabilities can be accessed through the direct USB API documented in our OEM data sheets, if you’re comfortable juggling endpoints and flushing pipes. However, if you’d prefer a higher-level application driver to access from your application, we offer two tiers of spectrometer device drivers. SeaBreeze is an open-source, cross-platform driver written in C++ which allows full control over all spectrometer functions on any chipset from Atom to ARM; you can download the full source directly from SourceForge and customize it to your heart’s content. For even more automation, OmniDriver provides handy object wrappers for Java, .NET, LabVIEW, MATLAB, Delphi and many other development environments.

Finally, if you don’t want to write code at all, try OceanView, our full-featured desktop spectroscopy visualization and analysis application suite. OceanView provides automated Wizards to walk you through each step of common spectroscopy measurements like absorbance and Raman, plus one-click access to standard laboratory functions like strip charts, colorimetrics, peak finding, and streaming data collection. You can even devise your own post-processing algorithms in the drag-and-drop visual schematic view, pipelining your feed from acquisition to answer to aggregate.

**Engineering Support, Production Capability and Vertical Integration**

Throughout the process of developing a solution for your product, Ocean Optics has a team of dedicated engineering resources available to assist your development. We know time to market is often one of the most important drivers for your business and we are ready to help you accelerate your process. Whether your needs are mechanical or electrical, software or hardware, we have the resources to help turn your product dream into a reality.