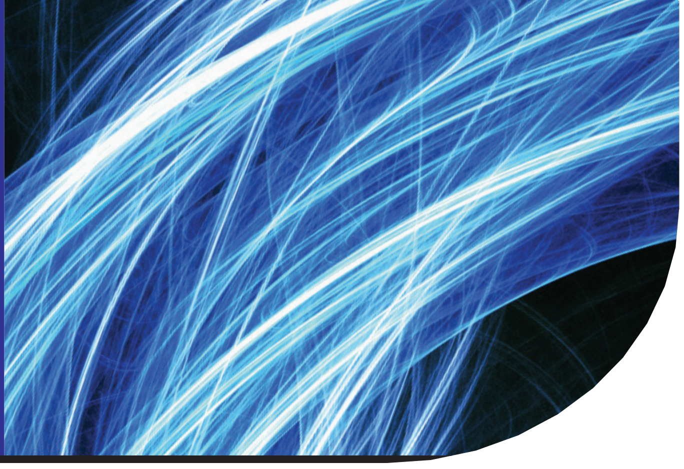
Spectroscopy Focus



How to Choose the Right Miniature Spectrometer

Choosing the right miniature spectrometer is very application-dependent, so there are a few questions that need to be asked. What are you trying to measure and why? How fast do you need measurements? Where is the sample and who will be operating the instrument? The design also involves money, so it is important to have a cost target for the system in mind as well.

To configure a spectrometer, there are some important choices that need to be made, such as the choice of wavelength range, optical resolution and system sensitivity. The optical bench directs broadband (white) light through a narrow entrance slit onto a diffraction grating and focuses the spectrum onto a detector array. The wavelength range will depend on the groove density of the grating and the details of the bench and detector.

> ***"… the gratings in most miniature spectrometers are fixed in place to ensure long-term performance and stability"***

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WAVELENGTH RANGE AND GRATINGS

The wavelength range is determined by the grating. With each grating, you consider its groove density (which helps determine the resolution), its spectral range (which helps determine the wavelength range) and its blaze wavelength (which helps determine the most efficient range). Instead of the gratings rotating as they do in instruments such as scanning monochromators, the gratings in most miniature spectrometers are fixed in place to ensure long-term performance and stability. A grating must be specified for each spectrometer.

CHOOSING THE RIGHT GRATING

The groove density (mm-1) of a grating determines its dispersion, while the angle of the groove determines the most efficient region of the spectrum. The rule of thumb is this: The greater the groove density, the better the optical resolution possible, but the smaller the spectral range. The spectral range is the dispersion of the grating across the linear array. The spectral range (bandwidth) is a function of the groove density and does not change.

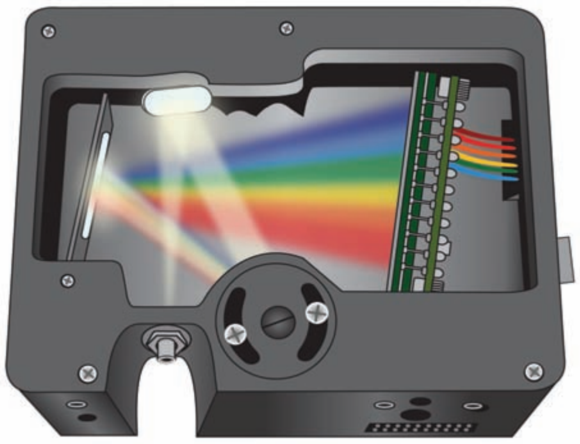

Figure 1: USB Bench

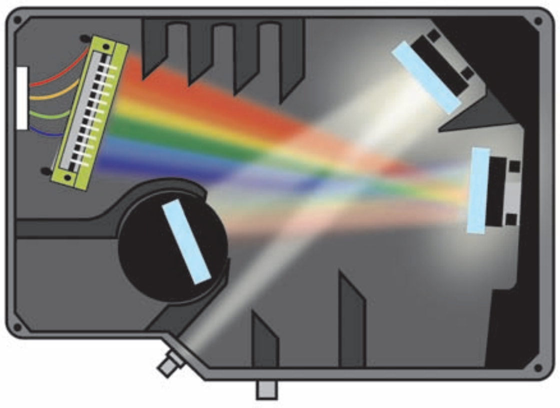

Figure 2: HR Bench

For example, in the 'USB' bench (*Figure 1*) in an Ocean Optics USB4000 Spetrometer, a 600 line mm-1 grating will cast a ~650nm spectra across the active area of the detector. So, for example, you can choose a spectral range from 200-850nm, or a spectra from 300-950nm. If you use a 1200 line mm-1 grating, then the light is diffracted at twice the angle and the detector will intercept half the wavelength range. The light is spread out over twice the angle, so it is half as bright and the signal will be half as great. With everything else held constant, the optical resolution would be twice as fine.

CHOOSING A LARGER BENCH FOR HIGHER RESOLUTION

If you choose a larger bench, you can also get higher resolution and less wavelength range. The 'USB' bench is a 42mm focal length design. The 'HR' bench (*Figure 2*) is a 102mm focal length design. In the 'HR' bench, the same 600 line mm-1 grating would yield a range of ~430nm and resolution that is 66% finer. Of course, the signal is lower because of the higher resolution. The other trade-off with the longer focal length is size and weight.

DETERMINING OPTICAL RESOLUTION

The optical resolution, measured as Full Width Half Maximum (FWHM) of miniature spectrometers depends on the groove density of the grating and the width of the entrance aperture (slit width or fibre diameter). In selecting these components, consider two trade-offs: First, the optical resolution improves as the groove density of the grating increases, but at the expense of spectral range and signal strength. Second, the resolution improves as the slit width or diameter of the fibre decreases, but at the expense of signal strength. For example, in an Ocean Optics HR4000 Spectrometer, a 100 micron slit will have an optical resolution of 14.0 pixels FWHM. Decreasing the slit width to 50 microns will improve the optical resolution to 7.4 pixels FWHM, but with the trade-off that there will be ~50% as much light. As the slit width decreases it approaches the diffraction limits and the improvement in resolution begins to diminish. So, going from a 50 micron slit to a 5 micron slit in the HR bench only improves resolution by a factor of 3.7 (instead of 10X).

FIRST AND SECOND ORDER EFFECTS

Light striking the grating is diffracted into multiple angles. The angles are whole-number multiples or orders that vary with wavelength. So, for example, first order light at 200 nm will be diffracted at angle #1, and also at angle #2, which is exactly twice as large as #1. Angle #2 is also the same as the first order angle taken by light at exactly twice the wavelength, or 400nm. If the application requires measurements at 400nm, and 200nm light is also present,

Figure 3: Linear Variable Filters

then the signal at the pixel in question will include contributions from both wavelengths. If, on the other hand, there is no deep UV light, then only 400nm will be detected. The second order light is usually removed by using filters. These filters have a transmission band and a blocking band to restrict radiation to a certain wavelength region. These filters are installed permanently inside the optical bench. Alternatively, linear variable filters (*Figure 3*) can be designed to match the dispersed spectra and provide the right blocking at each pixel in an array. The trade-off is that these linear variable filters are designed and fabricated for a particular bench, grating and starting wavelength so the options for adjusting spectra range are lost.

DETECTORS

Figure 4: Silicon CCD Detector

Detectors are chosen for several design features. Semiconductors are used to capture photons through absorption and convert them into current. The absorption band of silicon detectors (*Figure 4*) allows for good sensitivity over the UV, VIS and short wave NIR region (from as low as 160nm to as high as 1100nm). InGaAs detectors (*Figure 5*) generally work well from 900nm and higher. The upper wavelength range is 1700nm, but specially doped InGaAs can be used to extend that range to 2100 or 2500nm. The material of choice for mid IR range is Mercury Cadmium Telluride (HbCdTe).

PHOTODIODE DETECTORS

The effective range for detectors also depends on architecture. The simplest design is called a photodiode array. Each diode in the array is connected to readout circuitry that occupies a position next to the array. The diodes are supplied with a bias voltage, and photons that are absorbed by the silicon generate a current. The sampling circuitry generally features a sample and hold scheme and the ability to strobe through the row of detectors to acquire the voltage signal from each pixel. The stream of analogue signals is amplified and converted to digital information by external circuitry.

Figure 5: InGaAs Detector

CCD DETECTORS

The interest in imaging detectors led to the invention of the CCD or charge coupled detector. Here the photodiode is covered by a transparent capacitor that accumulates the signal during a length of time called an integration period. The advantage in 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 their polysilicon gates or capacitors absorb UV light, and so CCDs generally do not respond to light much below 350nm. There are two remedies to this problem. The CCD array can be coated with a phosphor, which absorbs UV 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 back side. This exposes the photodiodes to the UV light and the resulting device is significantly more sensitive to UV that the phosphor coated types.

SPEED OF ELECTRONICS, WELL DEPTH AND SIGNAL TO NOISE

Detectors are also characterised by the speed of their electronics, their well depth, sensitivity and signal to noise. Generally, detectors designed for imaging applications are optimised for speed. The ILX511 detector is a 2048-pixel linear CCD detector used in the USB2000+ (*Figure 6*) and can capture and transfer full spectra (2048 wavelengths) in 1 millisecond over a USB 2.0 port. The S7031 detector is a FFT-CCD detector used in the QE65000 (*Figure 7*) and is 16x slower than the ILX511, taking 8 milliseconds to acquire and transfer full spectra (1024 wavelengths). The well depth is the number of electrons that can be stored in the capacitor. The CCD capacitors are fully charged at time zero (equivalent to dark). If the quantum efficiency is 100%, each photon striking the surface depletes 1 electron from the well. When the well is fully depleted it stops responding to photons. The arrival of photons on the detector is a random process. This random shot noise ultimately limits the signal to noise of the measurement. The total noise or random variation is the sum of the shot noise, equal to the square root of the number of photons, combined with the dark noise and readout noise. When signals are high, as when the spectrometer is being used to measure light, the signal to noise is essentially equal to the shot noise. When the signal is low, as when a dark spectrum is being recorded, the noise is equal to the noise on the dark signal + the readout noise (coming from the electronics). The ratio of the maximum signal to the dark noise is called the dynamic range. A deep well detector will have a greater dynamic range than a shallow well. For example the dynamic range of the ILX511 is about 1300:1. The dynamic range of the S7031 is about 25000:1. This also means that it takes more photons to get a full-scale signal with the S7031 than with the ILX511. In fact, well depth and dynamic range are inversely proportional to sensitivity. In most applications it is desirable to maximize signal to noise, and the best detector depends on the type of light being sampled. If a transient event is being measured - for example, an arc from a xenon flash - then a high dynamic range detector is desirable. If the light is continuous, then in a given time frame the signal averaging of the fast shallow well detector will equal the performance of the slower deep well device. If the signal is very low, then the comparison of the signal to the readout noise must be evaluated. Generally, the shallow well device will be best.

COOLED DETECTORS FOR LOW LIGHT LEVEL APPLICATIONS

For low light levels, cooling the detector will lower the dark current and also the noise on the dark current. Signal to noise will be improved, and the ability to integrate signals for longer time periods is also made possible. Thus, the ILX511 shallow well detector will outperform the S7031 detector operating at room temperature when looking at low light levels. However, the S7031 features a built-in Peltier cooler and if it is used near 0°C, then it will have better performance than the ILX511. The trade-off here is the cost, power consumption and size of the Peltier cooling circuitry.

CONCLUSION

There are many things to consider when you configure a spectrometer and selecting design criteria involves accepting tradeoffs. The optimal configuration depends entirely on the application so before you can make good choices about hardware, you must understand your needs. The key is to learn system requirements early in the design process and rank the list: is performance more important than cost, or is a balanced approach preferred? As the Rolling Stones say, you cannot always get what you want. But when it comes to spectrometers, if you understand your requirements and consider the design tradeoffs, you can get what you need.

Figure 6: USB2000+ Spectrometer

Figure 7: QE65000 Spectrometer