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Polytec Technical series

Spectrometer design Transmission vs. reflection

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When astronomers envisioned the next generation spectrometer for their 21st century telescopes, they demanded the best performance and a robust design that could offer years of consistent service. Traditional spectrometer designs based on surface relief (SR) reflection gratings had been the standard workhorse for many decades. These astronomers recognized the limits of conventional reflection spectrometers with 2D surface scattering structures and the superior performance of transmission spectrometers based on 3D volume scattering structures, otherwise known as volume phase holographic (VPH) gratings.

Polytec engineers recognized the significance of this advancement in spectroscopy and incorporated VPH gratings into their spectrometer designs to deliver the best performance for their process analytical customers. With VPH technology engineered into the heart of every spectrometer, process specialists can relax knowing that their process monitoring and control is accurate, reliable, cost-effective, and uses superior technology integrated into field-proven process spectrometers. This brief introduction to spectrometer design compares transmission and reflection layouts, the two most commonly used designs. More specifically, transmission spectrometers such as Polytec's real-time PSS spectrometers have significant advantages in performance over reflection designs including maximum sensitivity, insignificant scattered light, and uniform optical resolution at the theoretical limit.

Czerny Turner spectrometer

Transmission spectrometer



Introduction to spectrometer design

A spectrometer's purpose is to measure the "amount of light" at specific and selected wavelengths. In other words, a spectrometer selectively quantifies each color of the rainbow. Today's spectrometers incorporate specific optical components including input and collimating optics, a dispersive element which is usually a diffraction grating, and focusing optics that direct the spectrum on to the detector array that bins the amount of light at each wavelength. The spectral resolution (the minimum wavelength separation needed to distinguish two narrow-band spectral lines from each other) and the wavelength range are two critical specifications for a spectrometer. Additional specifications are also important, including sensitivity, f-number, signal-to-noise ratio (SNR), size, cost, speed, linearity, and robustness (mechanical and thermal stability).

Transmission vs. reflection

The two most commonly used designs are the Czerny Turner (CZ) spectrometer (usually based on a reflective grating and mirrors) and the transmission grating spectrometer.

The major concerns for CZ type spectrometers include stray light (from imperfections of the grating), lower throughput of the system (due to the reflective grating) and the lower reflectivity of mirrors (compared to the transmission of lenses). Mirror-based systems, such as CZ type spectrometers, typically have optical errors such as defocusing, chromatic aberration, coma, spherical aberration and astigmatism. These are hard to compensate for overall wavelengths and usually require additional optical components such as aspheric optics or holographic optical elements.

Transmission spectrometers utilizing VPH gratings have a higher diffraction efficiency than reflective CZ type spectrometers. Not only do VPH gratings have higher diffraction efficiencies but they also lack the optical errors found in reflective CZ type spectrometers and have a very uniform performance over all wavelengths.

F-number, numerical aperture, etendue and resolution

The term f-number is used to describe the capability of an optical system to gather light. Another commonly used term is the numerical aperture (NA) which specifies the "opening angle" an optical system accepts. F-number and numerical aperture NA are inversely related. The equation shows that the larger the numerical aperture (NA), the smaller the f-number will be:

$$f#=\frac{1}{(2 \text{ NA})}$$

Etendue combines the NA and the (effective) area of the entrance slit to define how much light an optical system can couple into a spectrometer. Unfortunately, etendue and spectral resolution are two opposing parameters



that must be optimized for specific applications. A spectrometer's resolution is often measured using a monochromatic light source (e.g. laser) and scaling the Full Width at Half Maximum (FWHM) of that peak. Theoretically, the limit to the spectral resolution is the diffraction limit, but in most compact spectrometers, aberrations in the optics inside the spectrometer (the lenses/mirrors and grating) are the practical limiting factors. This optimization is accomplished by decreasing the opening angle (NA) and using a tiny entrance slit. By taking this approach, only a small portion of the available light gets to the detector, leading to low photon throughput and as, a consequence, a low signal-to-noise ratio (SNR).



Several examples of trade-offs between etendue and numerical aperture (NA) are shown below.

Advantages of a transmissive design

The major advantage of a transmission grating spectrometer compared to a reflective one is the higher throughput. The most significant contribution to this increased throughput comes from the higher diffraction efficiency of VPH gratings. Further adding to the throughput, high-performance antireflection (AR) coatings minimize Fresnel losses. Reflective gratings (and the mirrors used in a CZ spectrometer) have lower performance due to surface losses in the reflection process. In the design of VPH gratings, there are also more parameters available to optimize the grating for its intended wavelength-range. The efficiency, when plotted against wavelength, is quite uniform for VPH gratings. Reflective gratings used in CZ spectrometers are optimized for a specific wavelength. Their effectiveness decreases quite significantly away from that wavelength.

Process spectroscopy and the need for ruggedness

A common practice when using high-resolution CZ based spectrometers is to tilt the grating about a fixed axis to sequentially measure different spectral ranges. A CZ spectrograph can also be designed using a fixed grating. However, any tilt or rotation of the grating (e.g., induced by vibrations, shock, or temperature) will change the spectral range measured and the wavelength accuracy as well. In contrast, a VPH transmission grating is insensitive to its rotation, because there is no effect on the deflection angles. Transmission gratingbased spectrometers are therefore more stable and robust.

Spectrometer design summary

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Transmission grating based spectrometers offer advantages in complex measurement applications such as:

- Low light level (high throughput of the transmission spectrometer)
- Fast spectral acquisition for high temporal resolution
- High process stability with regards to variations in temperature or vibrations

A component-based spectrometer design makes all spectrometer components (especially the detector) accessible which simplifies the integration and maintenance of transmission spectrometers in a process environment. Integrators prefer spectrometer designs with substantial component accessability as it enables and optimizes their specific applications.





High performance

Polytec PAS NIR Spectrometer Systems

PAS spectrometers are designed for real-time industrial applications. Based on low noise diode array technology, precision optics and superior transmission grating design, PAS spectrometers are an ideal tool for fast and reliable data acquisition. Flexible integration in various measurement scenarios is enabled through the use of fiber coupled components.

PAS spectrometers are the optimal solution for NIR Process analytics.



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