

THE WASATCH ADVANTAGE



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Increasing demand for lightweight, portable instruments, along with improvements in optical design and manufacturing technologies, is leading to the development of a new generation of ultra-fast Raman spectrometers. New opportunities in manufacturing process control, raw material identification, counterfeit detection, SERS applications, forensics, pharmaceutical QC, transportation security and many other areas are driving this growth. Many of these applications require maximizing data collection rate. When measurements must be made on a high-speed production line, milliseconds matter. In handheld platforms, time may not be the critical factor, but concerns over battery power consumption may drive spectrometer selection. Another application might require the detection of minute concentrations of a material of interest.

Each of these applications share two things in common – they would all benefit from a spectrometer design optimized for 1) the greatest possible *acceptance angle*, and 2) the highest possible *throughput*. All other things being equal, an instrument with greater throughput and a larger acceptance angle will be able to collect data faster, use less power, and detect lower sample concentrations than would an instrument with less throughput and a smaller acceptance angle. This paper will describe the key factors in spectrometer design that have the strongest influence on acceptance angle and throughput.

F-ratio

Light enters the spectrometer through a slit and is bound within the *acceptance cone*. The angle that the side of this cone makes with the optical axis is the acceptance angle, and is defined by the entrance F-ratio (f/#), which is the ratio of the focal length (F) to the diameter (D) of the spectrometer aperture (see **Fig 1** below). The F-ratio sets an upper limit on how many photons are given a chance to reach the detector. Since F-ratio is inversely related to the acceptance angle, this means that a lower F-ratio will allow more photons to enter the spectrometer than would a similar instrument with a higher F-ratio. It determines the number of photons reaching the detector more fundamentally and with greater impact on system performance than any other aspect of spectrometer design.

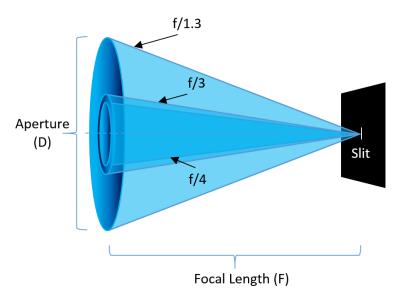


Fig 1. F-ratio determines how much light can enter the spectrometer – lower F-ratios allow more light.



Optical Losses

Once the photons make it into the spectrometer, there are several optical surfaces they must interact with before they have a chance to arrive at the detector. Each of these interactions provides an opportunity for photons to be lost, or worse, scattered and become a source of stray light that degrades instrument performance by decreasing sensitivity. The goal of the spectrometer designer should always be to minimize these sources of loss, thereby maximizing system throughput. Several design choices will have a strong influence on throughput:

- 1) Use refractive optics whenever possible. Reflective optics tend to absorb and scatter more light, and are more difficult to align as compared with refractive optics. Also, if a refractive element and a reflective element both suffer from the same manufacturing surface defect, the reflective element will produce twice the wavefront error as compared to the refractive element.
- 2) Minimize the total number of optical elements.
- 3) Use a diffraction grating with the highest possible efficiency.

The detector selected will also influence system throughput, as it contributes to losses as well. But a discussion of sensor quantum efficiency goes beyond the scope of this paper. In the following comparison of two spectrometer designs, we will assume the same sensor is used in both instruments.

The classical Czerny-Turner or Crossed Czerny-Turner (CCT) optical design consists of a reflective mirror to collect and collimate the incoming light, a reflective diffraction grating, and another reflective mirror to focus the diffracted light onto the detector. Application requirements that limit the physical size of the spectrometer to a small fraction of a cubic foot do not benefit from the one advantage this design offers: large mirrors can be made at much lower cost than large lenses can. However, several spectrometer manufacturers are still offering scaled down versions of the CCT design. But they cannot compete with the superior throughput of a well-designed axial refractive spectrometer.

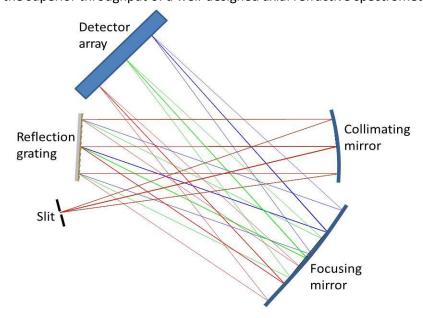




Fig 2. The Crossed Czerny-Turner (CCT) Design – a good choice for very low light applications where physical size is not a concern.

The axial refractive design employs entirely refractive optics, and maintains good symmetry about the optical axis. This means any aberrations present will be less impactful on system performance, and optical alignment can be achieved with tighter tolerances. A single lens with anti-reflection coatings typically has significantly higher throughput (% transmission) than a mirror (% reflectance) with conventional reflective coatings. If the number of lenses is minimized in the axial refractive design, the amount of light lost will be significantly less than in a competing reflective design. Consider a typical CCT that employs two mirrors for collimating and focusing the incoming light as in **Fig 2** above. Conventional reflective coatings yield at best about 90% average reflectance, so with only 2 surfaces, the system throughput is already down to 81%.

In the optimized axial refractive design, shown in **Fig 3** below, the fewest number of lenses is used to collimate and focus the light. The f/1.3 Wasatch design incorporates anti-reflective coatings that limit reflection losses to less than 5% for a system transmission of more than 95%. This design is also optimized to reduce aberrations below the diffraction limit. The off axis nature of the CCT design on the other hand makes diffraction limited performance significantly more challenging and costly to achieve.

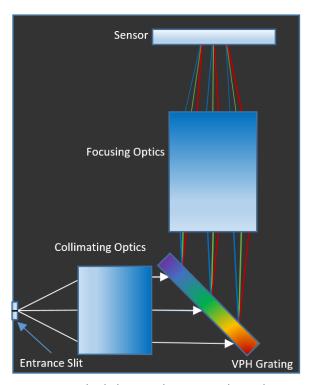


Fig 3. The Axial Refractive Design – an ideal choice where size, throughput and sensitivity matter most.



The last component that has a significant influence on system throughput is the diffraction grating. This is the element responsible for spreading the incoming light into its component parts. Here again, improvements can be made in system throughput if a refractive grating is used rather than a reflective one. Reflective surface gratings are prone to surface damage, oxidation, and contribute to stray light more than refractive gratings in general. A Volume Phase Holographic (VPH) grating further reduces optical losses by encapsulating the diffractive element between two layers of optical glass or fused silica.

The Wasatch VPH grating is made using dichromated gel technology, which exposes a photosensitive gelatin to an interference pattern produced by a laser and beamsplitter. The interference pattern produces a very smooth and periodic variation in refractive index within the gelatin, which is chemically developed, baked and then imbedded within optical epoxy and fused silica or another optical glass, depending on transmission requirements. This process results in a much higher diffraction efficiency than conventional methods. Comparing two gratings designed for the same bandpass region, Wasatch VPH gratings typically achieve an average efficiency of ~80%, while standard gratings achieve at best ~45-65% as shown in **Fig 4** below.

Standard holographically blazed reflection grating (Al coated)

Volume-phase transmission grating

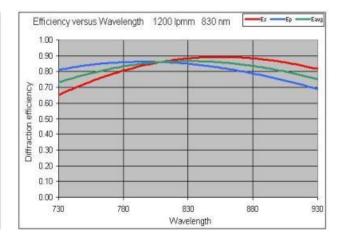


Fig 4. The advantage in diffraction efficiency of a Wasatch VPH transmission grating over a standard reflection grating.

So the CCT spectrometer equipped with a standard reflective grating can yield at best a system throughput of $\sim 0.81 \text{ x} \sim 0.65 = 52\%$, while the axial refractive design equipped with a Wasatch VPH grating yields $\sim 0.95 \text{ x} \sim 0.80 = 76\%$ system throughput.



Adding it all up

Typical CCT F-ratios are in the range of f/3 to f/4, while the Wasatch axial refractive design is optimized at f/1.3 (refer again to **Fig 1**). Since the amount of light that can enter a spectrometer goes with the *inverse square* of the F-ratio, we can write the following to describe the % of light that can enter the CCT design (assuming the best case f/3) compared to that of the Wasatch design: $(1.3^2/3^2) = 18.8\%$. Or, the Wasatch design collects more than 5 times the light that the CCT design collects. As stated earlier, F-ratio drives system performance with greater impact than any other design parameter. This real-world example shows that clearly. In comparison, the added losses due to choosing a reflective design over a refractive one pale in comparison to the all-important F-ratio.

Consider an application which allows a maximum integration time of 50msec. **Fig 5** shows how peak heights compare between the Wasatch f/1.3 system and an f/4 CCT design of similar size (Cyclohexane is used in this example).

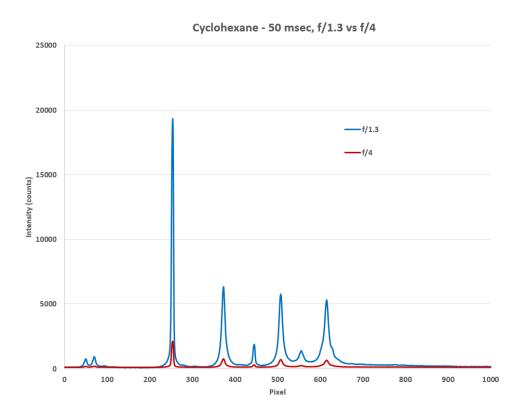


Fig 5. Impact of F-ratio on signal intensity for a fixed integration time.

If the application requires that very low sample concentrations be detected, a low F-ratio and refractive optics provide similarly superior performance over the higher F-ratio alternative. Due to the additional losses incurred by using optical fiber for coupling, it's generally preferable to free-space couple the spectrometer, especially for low-signal applications. If a fiber and external probe must be used, the F-

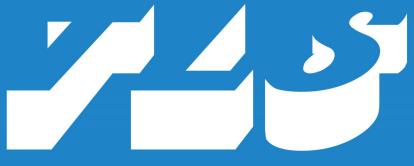


ratio of the probe will limit the acceptance cone into the spectrometer unless they are F-ratio matched. **Table 1** shows how the Limit of Detection (LOD) for Isopropanol varies with F-ratio. LOD values are given in % Isopropanol concentration. 120mW laser power at 785nm was delivered to the sample in each case, with 500msec integration times.

	f/4 spectrometer	f/1.3 spectrometer	f/1.3 spectrometer	f/1.3 spectrometer,
	with fiber & f/2.2	with fiber & f/2.2	with fiber & f/1.3	free-space
	probe	probe	probe	
LOD (%	0.13%	0.12%	0.07%	0.025%
Isopropanol)				

Table 1. Impact of F-ratio on Isopropanol Limit of Detection.

No spectrometer on the market offers an F-ratio to compete with the Wasatch f/1.3 design. With more photons collected at the aperture by far than competing units (500% more than competing f/3 designs, and 900% more than f/4) and fewer sources of loss to provide greater system throughput, the Wasatch Advantage is clear.



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