Enhanced Chemical Identification Using High-Throughput Virtual-Slit Enabled Optical Spectroscopy and Hyperspectral Imaging

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INTRODUCTION

There is a growing opportunity for the use of non-invasive or stand-off identification of chemical species across the fields of Industrial Control, and Security and Defense, Environmental Monitoring, Process Analytical Technology, and Food Safety. One of the fastest growing techniques for performing this type of detection and identification is optical spectroscopy, a maturing technique (>$5B in global instrument sales in 2011) that is now seeing wide use outside of the laboratory, especially for Raman spectroscopy ($200M market in US by 2014). These techniques provide users with more accurate non-invasive identification of materials for a growing number of applications.

Until now, however, the extension of optical spectroscopy to a wider range of applications has been limited by a classic trade-off in traditional spectrometer design. Such a compromise prevents any single device from achieving both the high spectral resolution and the high signal level required to practically differentiate chemical species under many conditions in which the optical signal available for collection from the sample is limited.

This white paper describes proprietary HyperFlux optical spectrometer designs developed by Tornado Spectral around a core technology (the High-Throughput Virtual Slit, or HTVS) that eliminates the throughput vs. resolution trade-off found in other dispersive spectrometers and enables new applications. We also describe the HyperFlux's ability to enhance the performance of hyperspectral imaging systems.

OPTICAL SPECTROSCOPY

Spectroscopy in optics is the study of the different frequency or wavelength components (colors) of a light source, and using this information to deduce information about the material samples with which the collected light interacted. Variations in molecular structure correspond to different optical properties, creating unique spectroscopic "signatures" used to identify the materials under interrogation. The devices used to collect and identify the intensity of each wavelength of light in these signatures are called optical spectrometers, of which there are several types. This white paper focuses on the use of dispersive spectrometers since their speed and absence of moving parts make them the preferred choice over interferometric and scanning filter-based spectrometers for most commercial and military applications that require lower cost, speed, and ruggedization for deployment.

There are several types of optical spectroscopy, including Emission, Absorption, and Raman. Raman in particular is gaining traction across an ever wider range of applications. Raman spectroscopy exploits an effect where a small fraction of the laser light striking a material will scatter at different wavelengths (the Raman effect) than the incoming laser wavelength, while the rest of the light is scattered with no change in wavelength. This Raman technique has shown great promise for high accuracy in differentiating materials using portable and robust spectrometer configurations outside of the laboratory. Despite the growing use of the technique, until now its usefulness has been limited by the faintness of the Raman-shifted signal.

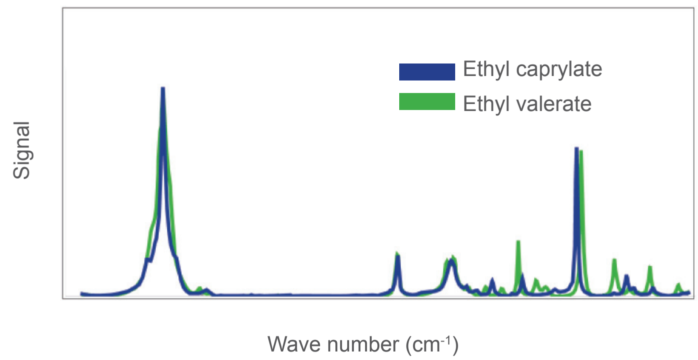

Figure 1. The Raman spectra of these molecularly-similar materials demonstrate the importance of spectral resolution and signal strength to discrimination between samples

OPTICAL DISPERSIVE SPECTROMETER PARAMETERS AND THE CLASSIC TRADE-OFF BETWEEN RESOLUTION AND THROUGHPUT

Typically, a spectrometer's performance is quantified by a few critical parameters including the optical bandpass (the range of detectable wavelengths), the spectral resolution (the narrowest spectral feature that can be independently resolved), and the optical throughput (the percentage of light entering the device which reaches the detector). These three key spectrometer parameters then combine with the optical collection system that delivers the light from the sample to the spectrometer. Along with the detector efficiency, noise, and speed, complete performance of a spectroscopic measurement system is determined.

In many applications the three key spectrometer parameters are all important. For example, higher spectral resolution can give a sharper view of the target spectrum, permitting a more detailed analysis. Higher throughput can provide a stronger measurable signal, improving the quality of the data. However, virtually all spectrometer designs available today include tradeoffs among these critical parameters.

Dispersive spectrometers function by incorporating some form of optical dispersive element such as a prism or grating that separates the incoming broadband light beam into its constituent wavelengths and projects the light onto the detector plane. (Note that while wavelengths of light are often presented as different "colors", a spectrum often includes wavelengths invisible to the human eye including infrared and ultra-violet wavelengths.) The light intensity of each wavelength contained in the spectrum is then determined by the intensity of light at different locations on the detector plane as determined by the relative positions of the dispersive element and the detector position.

The generally accepted technique to achieve higher resolution in a dispersive spectrometer is to use a physical slit to mask the image of the incoming beam before it passes through the dispersive element, which effectively narrows the position of each wavelength component of the projected spectrum on the detector plane. This is a simple and effective way of improving the spectral resolution, as shown in the figure below, but it comes at the high cost of wasting all of the light not passing through the slit.

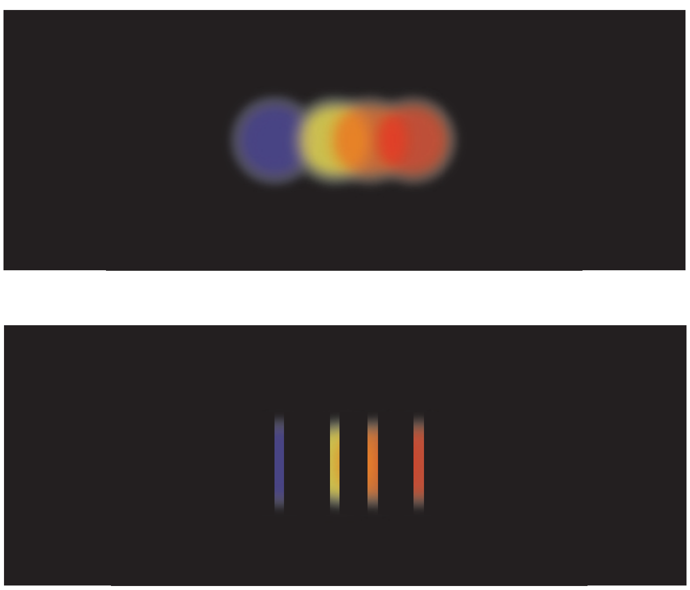

Figure 2. Representation of how a dispersed spectrum on a focal plane (top) is masked using a slit (bottom) to improve separation of wavelengths, resulting in better resolution at the cost of lost light

This wasted light can often constitute 80-95% of all the light entering the spectrometer (depending on the desired resolution). Unfortunately, this tradeoff between resolution and throughput is not simple to overcome. Due to the conservation principle of "Étendue" in an optical system, an improvement cannot be gained by using focusing optics to create narrower beams, as any increased focusing to increase throughput at the slit will be countered by a greater divergence at the exit, cancelling out any anticipated advantage.

The Étendue of an optical system is a 2D geometrical measurement of the light collected given a finite source area and a finite entrance pupil area. Mathematically it is represented as,

$$E = A_{EP}\,\Omega_s,$$

where AEP is the area of the entrance pupil and Ωs is the solid angle of the source as seen by the entrance pupil. The solid angle of the source is proportional to its area and is represented as,

$$\Omega_s = \int_{\varphi}\int_{\theta} \sin(\theta)\,d\theta\,d\varphi.$$

The limits on θ and φ are determined by the width and height of the spot and are directly related to the width and height of the entrance pupil. The width of the spot may be reduced to provide higher spectral resolution but in order to keep the entrance pupil area the same, the height of the spot must increase by the same amount. In other words, θ and φ are freely variable parameters, and as long as the entrance pupil area is unchanged the Étendue will remain the same and there will be no throughput loss.

Dispersive spectrometer designers have accepted the losses due to a slit and focused their efforts to improve spectrometers by optimizing the efficiency of the remaining optical elements, using more sophisticated detectors and electronics (e.g., liquid or thermal-electrically cooled detectors), dispersive elements (e.g., volume holographic gratings) and reflective coatings (e.g., stacked dielectric coatings with $<2\%$ reflection losses). In fact, many spectrometer manufacturers quote their relative throughput by ignoring the slit loss because it is considered to be a "constant" inherent to all spectrometer designs. The full potential of optical spectrometers, however, is only achievable by solving this full order-of-magnitude loss caused by the slit, as is achieved with the development of the HTVS and its incorporation into all of Tornado Spectral's spectrometer designs.

THE HTVS AND TORNADO SPECTRAL'S HYPERFLUX SPECTROMETER TECHNOLOGY

Conventional spectrometers use a narrow entrance slit to achieve higher resolution at the cost of throughput. Tornado's proprietary designs use a patented specialized technology to modify the shape of the beam in the spectrometer with >90% total optical throughput. The input aperture is anamorphically converted into a slit-like shape without violating the Étendue principle. The classic trade-off between resolution and throughput in a dispersive spectrometer is eliminated using HTVS technology.

The optical foundation of the HyperFlux spectrometers uses a comparatively large input aperture (for maximum throughput) in combination with a series of specially configured mirrors, lenses, and other elements. These components act to compress, reformat, and then expand the light beam, with the end result of narrowing the input aperture along the dispersion axis while preserving total flux, delivering dramatic performance improvements; Tornado's technology narrows the input beam to the same effect as a traditional slit, but conserves flux at the focal plane by reformatting the beam.

Beam reformatting is not a new concept in spectroscopy. It has been previously observed that the Étendue principle confirms that the conservation of flux on the image plane (e.g., at the slit) is not violated if that image is rearranged to trade horizontal for vertical flux in the image plane. Such image "slicers" have been proposed as early as 1938 but the implementation of such designs has not been commercially practical for several reasons. Instead, Tornado's spectrometers incorporate a novel approach where the reformatting takes place in the unfocused "pupil" or "Fourier" space rather than in image space. This proprietary approach provides a simpler and more practical implementation to reformat the beam. When the beam in "pupil" space is focused, the corresponding image is now in the shape of an elongated oval, preserving all of the light while providing the narrower spot image required for high resolution and preserving the imaging f/# as described by the Étendue principle:

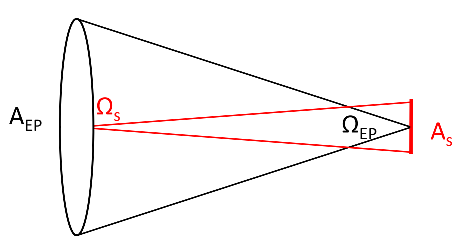

Figure 3. HTVS manipulates the geometrical description of the Étendue but keeps it constant to preserve throughput

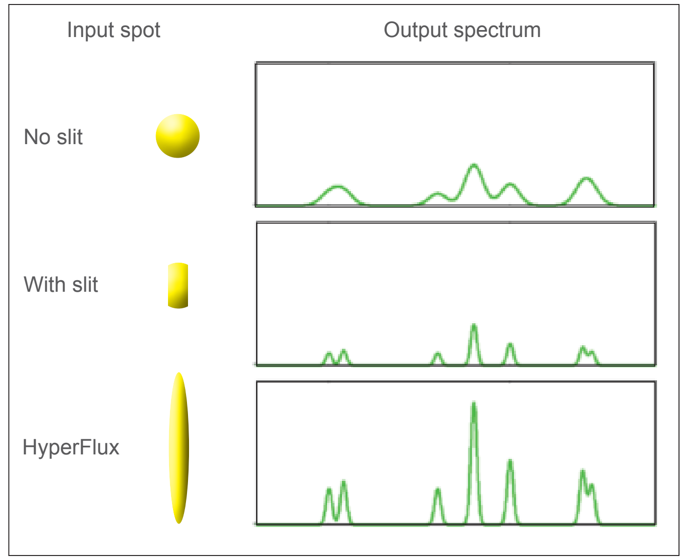

Figure 4. The relative shape of the beam and corresponding spectrum from the traditional slit and the HyperFlux spectrometer

Comparison to other techniques to overcome the classic trade-off

Researchers and engineers have devised various methods to increase throughput while maintaining resolution without the performance achieved by HyperFlux, either by using fiber bundles or optical slicers, or coded apertures.

Fiber bundles convert an input spot into a line of light by collecting light in a tightly packed arrangement of fibers and fanning them out into a slit-like line. However, a large portion of the fiber bundle cross-sectional region consists of cladding area between the packed fibers, and any incident light on this cladding surface is lost, resulting in significantly lower transmission than HyperFlux. Also, silica fibers have significant absorption in the UV and mid-to-long IR wavelength regimes, limiting their use compared to the capabilities of HyperFlux.

Image slicers are also technologies designed to help manage the resolution and throughput tradeoff. Image slicers work on a micro scale using a combination of small mirrors or waveguides to "chop up" a light spot in order to reduce the amount of light lost through an input slit. Light losses due to interstitial regions, the spaces between optical components such as lenses and mirrors, also reduce efficiency. Additionally, image slicing components are sensitive to tolerances and require very high precision alignment, making them impractical for use in commercial products.

Another method for improving light throughput with high spectral resolution is with the use of **coded**

apertures, which uses a two-dimensional pattern of holes to cast a shadow of the light onto the detector, which when combined with computational algorithms can determine the spectrum of the incoming light source. This approach requires very high tolerances for precise image quality, more expensive array detectors, and computational power, while only approaching a maximum throughput of 50%.

Compared to all of the above approaches the HyperFlux spectrometers, using the HTVS approach, deliver higher performance using simpler optics that can be applied to a larger range of requirements.

WIDE APPLICABILITY OF THE HTVS-ENABLED SPECTROMETER CONCEPT

The HyperFlux designs are unique in that the HTVS technique used relies exclusively on reflective components to achieve the reformatting, avoiding the introduction of any additional glass elements or fiber optics. This prevents any undesired material dispersion or absorption and allows the technology at the core of the HyperFlux spectrometers to be applicable across all wavelengths from Ultraviolet (UV) through Long Wave Infrared (LWIR).

As mentioned previously, while the HTVS technology can benefit any form of high resolution optical spectroscopy, there is a particular opportunity to dramatically enhance the performance of Raman spectroscopy systems. Raman spectroscopy is gaining more and more interest as an analytical technique to complement or replace absorption optical spectroscopy, mass spectroscopy, and liquid and gas chromatography. This intense interest is due to the strong specificity of the Raman signature of many materials. However, the already weak Raman signal is often lost because of the poor throughput of traditional slit spectrometers. Tornado's spectrometers overcome this performance shortfall by ensuring that the signal is not lost to the spectrometer itself.

The graph below shows a comparison of the Raman spectrum of kerosene as measured with Tornado's HyperFlux spectrometer and two competitors.

- Unlike HyperFlux, both competitors use TE-cooled detectors (requiring power supplies and internal fans)
- HyperFlux resolution is ~2x better than Spectrometer A, and is approximately the same as Spectrometer B despite the fact that the integration time of HyperFlux is only 1/5 of the integration time of Spectrometer B, demonstrating HyperFlux's much higher throughput

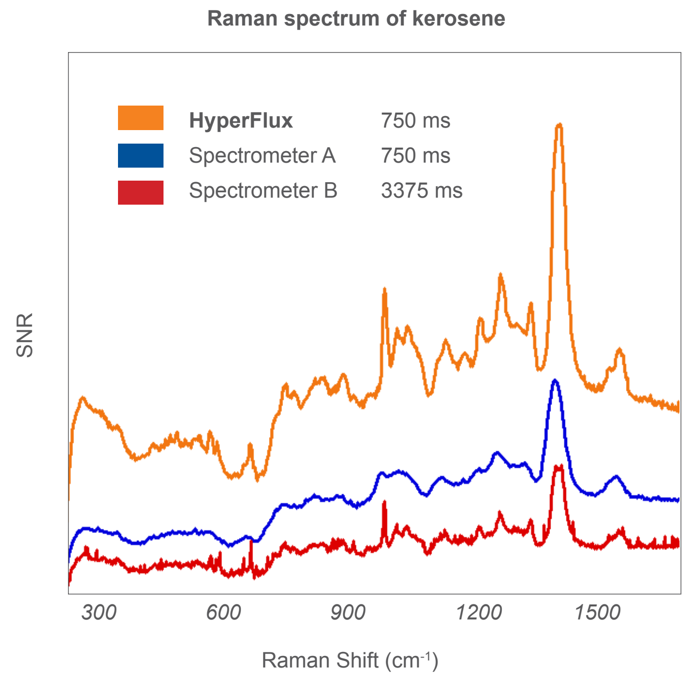

Figure 5. The Raman spectrum of kerosene shows dramatically greater detail within its specific spectral signature using HyperFlux than with other spectrometers

HYPERSPECTRAL IMAGING

Most spectroscopy is performed on homogenous or quasi-uniform material samples but there are applications where the identification of variations in spectral signatures across a given sample area is necessary. When a spectrometer is configured to capture both the spatial variation and the corresponding spectral signature, such a system is referred to as a multi-spectral or hyperspectral imager, where hyperspectral refers to systems with much greater spectral resolution than multi-spectral.

Hyperspectral imagers come in many different configurations depending on the applications of interest. They range from high-speed and close proximity for quality control on the manufacturing assembly line to lightweight and high sensitivity for airborne monitoring and surveillance. In general, however, hyperspectral imaging systems on the market today have the same limitations and face the same constraints as non-imaging optical spectrometers; i.e. they compromise throughput for the sake of increased spectral resolution.

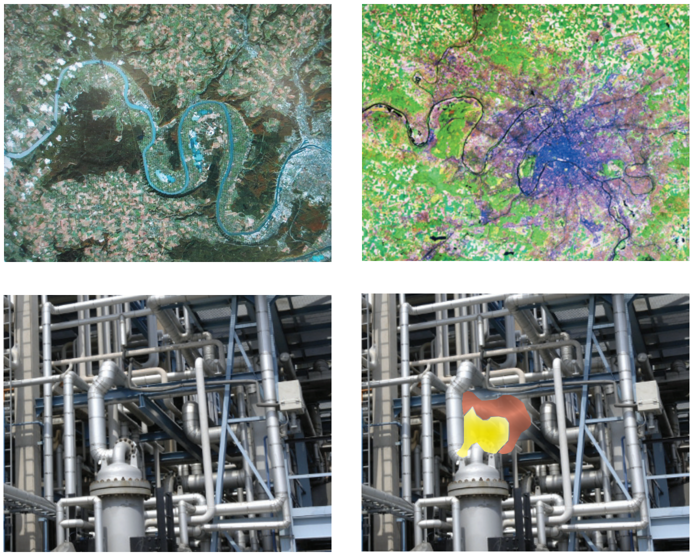

Figure 6. Applications for hyperspectral imaging include i) aerial observation of vegetation (color satellite {Top L} vs false-color hyperspectral {Top R}), and ii) industrial monitoring of gas leaks (color image {Bottom L} vs hyperspectral highlight of ammonia gas signature {Bottom R})

Applicability of HTVS to Hyperspectral Imaging

One of the non-intuitive aspects of Tornado's HTVS technology is that the reformatting process preserves relative spatial positions within the input aperture. This allows the same designs at the heart of HyperFlux to be applied to hyperspectral imaging, where the spectrometer may collect the spectra from hundreds or thousands of point sources across a line of view at the same time. As shown in Figure 6, each point along a line input will be both narrowed and elongated, improving throughout for a given spectral resolution without the use of a traditional slit in the spectrometer.

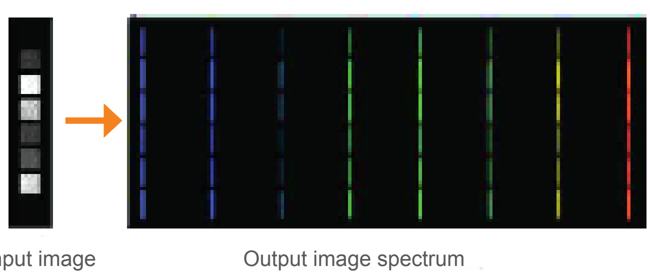

Figure 7: All spot sources (spatial pixels) in a hyperspectral imaging system can be reformatted simultaneously to deliver more light than an equivalent slit-based imager

This capability is validated by Tornado's S4 demonstration imager, which uses HTVS technology. A hyperspectral imager like the S4 can achieve the same spectral resolution as a traditional imaging spectrometer while using a wider slit, or can reach higher resolutions with the same slit width. In either case, the higher throughput can improve several performance metrics over common hyperspectral imagers.

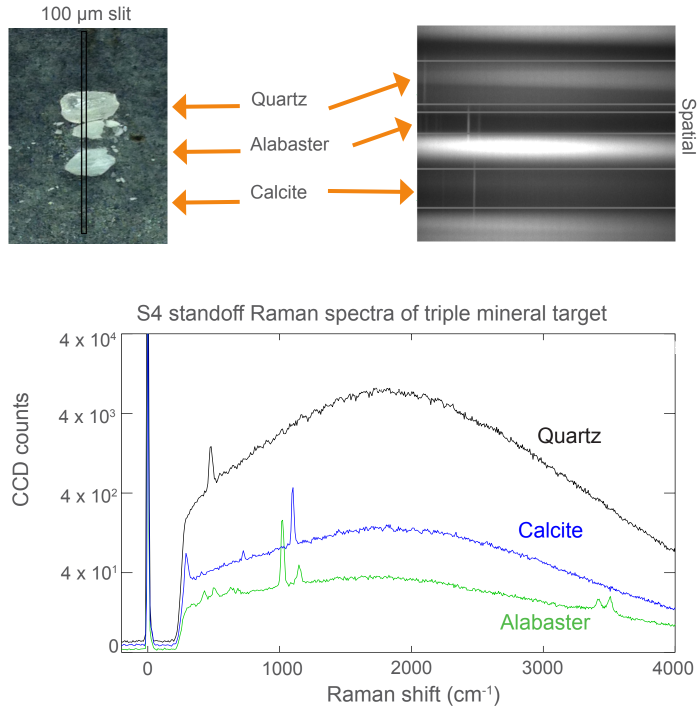

Figure 8. S4 hyperspectral prototype results showing three minerals scanned simultaneously in standoff Raman configuration

BENEFITS OF USING TORNADO'S TECHNOLOGY

The additional optical throughput at high spectral resolution is a benefit that can be translated into several different advantages to any spectroscopy systems.

Spectrometers:

- Collect higher quality data with higher resolution and/or higher signal strength
- Reduce acquisition times for a given source
- Compensate for weak light sources or input
- Enable new spectroscopy applications
- Reduce weight and cost by minimizing cooling equipment for detectors and lasers, and reducing the size and weight of collection apertures

Hyperspectral imaging:

- Increase the collected flux (and thus signal-to-noise ratio) from extended targets like smoke plumes, homogenous surfaces, and the atmosphere.
- Improve spectral discrimination for narrow-line sources such as Raman and LIBS emission, atomic emission, and molecular absorption bands.
- Discern faint spectral lines (both absorption and emission) against a broadband (e.g. daytime) background.

APPLICATIONS FOR HTVS-ENABLED SPECTROSCOPY

While nearly any optical spectroscopic application for material identification can benefit from Tornado's technologies, the following table describes how specific benefits apply to some sample applications:

Advantage	Needed For	Sample Applications
Increased spectral resolution	• Identifying samples with closely spaced spectral features • Discrimination between samples with similar spectral features	• Security screening • Threat detection • Forensic analysis • Material science
Detection of weak signals	• Low ambient light • Raman response (especially with limits on laser power) • Measurements taken at longer distances	• Stand-off detection • Trace sample detection • Aerial imaging with varying cloud cover • Radial velocity measurements
Short acquisition times	• Moving samples • Changing samples • Large number of samples	• In-line process monitoring • Security screening
Lower electrical power requirements	• High quality signal without use of a cooled detector	• Portable analyzers
No moving parts	• Rugged designs • Minimal calibration	• Portable systems for military and civilian applications
Lower weight	• Mobile sensing • Smaller volume	• Aerial imaging for fuel and weight-sensitive applications • Any portable system

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