

The Triplet Spectrograph – Spectrograph Design for the DXR Microscope and SmartRaman Spectrometers

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Summary

The Triplet Spectrograph used in the DXR microscope and SmartRaman spectrometers is of a unique design that enables it to support an unusually high spectral resolution relative to its overall wavelength range.¹ The Triplet Spectrograph is able to capture the full range Raman spectrum at 4 cm⁻¹ resolution in a single exposure using a fixed grating mount. Unlike more conventional designs, the Triplet Spectrograph provides optimal resolution and focus that is independent of the excitation laser wavelength. This Technical Note describes the design innovations and includes data to demonstrate performance.

Introduction

The DXR microscope and SmartRaman spectrometers are designed to be used in laboratories and industrial settings for routine yet rigorous analysis. This requires instruments that can deliver uncompromised spectral data, yet be easy to use, easy to maintain and come with low cost of ownership. Ideally a spectrograph for this environment should be able to capture the full Raman spectrum in one exposure. This minimizes collection time, avoids stitching artifacts and, by eliminating the need for a device such as a moving grating, simplifies the design and minimizes the need for maintenance. The spectrograph design should also deliver optimal performance with multiple excitation lasers.

A majority of Raman spectra are fully resolved at a spectral resolution of 4 cm⁻¹. Peaks that are useful for compound identification are found almost entirely within the range of 50 to 3500 cm⁻¹. We used these parameters to set the performance goals for the new spectrograph.

Triplet Spectrograph Design

Requirements

The fractional resolution of a spectrograph is defined as the spectral resolution expressed as a fraction of the overall wavelength range. It is a useful measure of the quality of the optics and is independent of the wavelength range chosen. The number of spectral channels is the reciprocal of the fractional resolution. In order to be able to capture a spectral range of 3450 cm⁻¹ at 4 cm⁻¹ resolution in a single exposure a spectrograph has to have a minimum of 865 spectral channels. As an additional challenge, the fractional resolution should ideally remain constant, even when the wavelength range is changed by changing excitation lasers, diffraction gratings and the grating angle.

Existing Designs

The conventional spectrograph for a dispersive Raman instrument is based on the Czerny-Turner configuration. While the Czerny-Turner spectrograph is a good choice for many applications, it suffers from fundamental limitations in spectral resolution. It is uncommon to see a Czerny-Turner-based Raman instrument offer more than 500 spectral channels without sacrificing numerical aperture. A further problem with the Czerny-Turner design is that the spectrograph grating contributes to the optical aberrations of the system through anamorphic magnification, and this changes as the working angle of the grating is changed. This results in the fractional resolution varying across the spectrum and with different excitation lasers.

Echelle spectrographs provide some benefits for dispersive Raman spectroscopy. An echelle is able to capture the full spectrum in one exposure and has no moving parts. However, they also have limitations. They are difficult to configure for use with more than one excitation laser. In addition, the stitched spectrum that they generate is subject to potential base line artifacts at the stitch points and large fluctuations in signal-to-noise across each segment of the stitched spectrum.

Key Words

- Low-maintenance Spectrograph
- Raman Spectroscopy
- Spectrograph Resolution
- Triplet Spectrograph

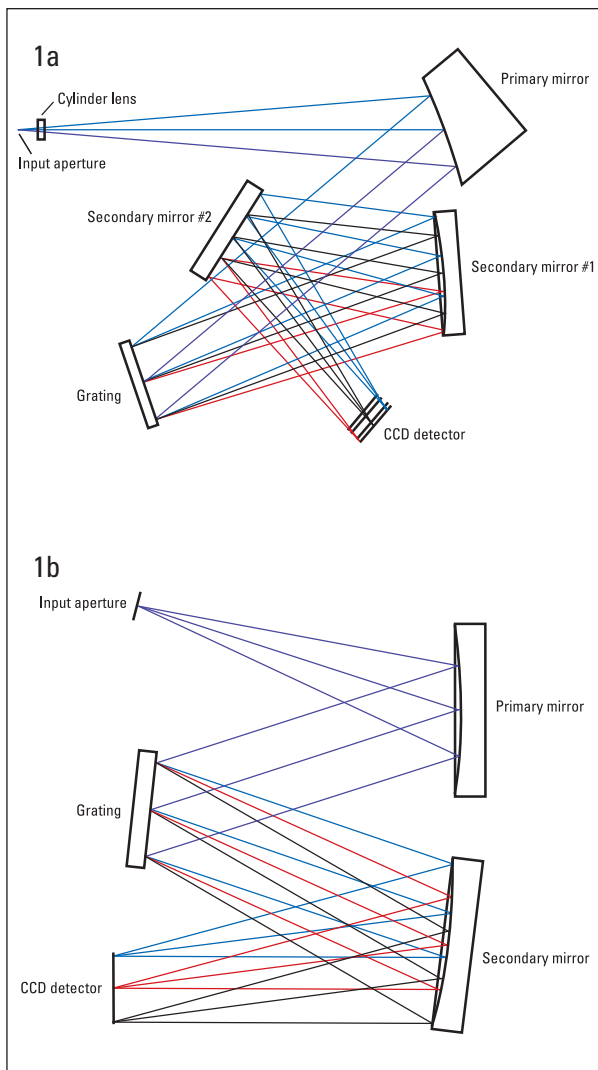


Figure 1a and 1b: Spectrograph Configurations. (a) Triplet Spectrograph; (b) Czerny-Turner.

The Triplet Spectrograph

The Triplet Spectrograph is a new design developed specifically for the DXR microscope and SmartRaman spectrometers. We have addressed the limitations of existing spectrograph designs by configuring the Triplet Spectrograph with an off-axis parabolic mirror to minimize aberrations in the primary optics (prior to the diffraction grating). This renders the spectrograph insensitive to changes in the anamorphic magnification of the grating. The design (Figure 1) also features a two-mirror secondary system that optimizes the focus of the beam at the detector across the entire frequency range, resulting in a system that greatly outperforms the single secondary mirror of a Czerny-Turner spectrograph and that is optimally focused at all excitation wavelengths. The net result is a spectrograph with a resolution that approaches 1000 spectral channels.

Spectrograph resolution is also affected by the number of detector pixels. Two narrow features in a spectrum are said to be resolved if they can be distinguished from a single broad feature. An example is shown in Figure 2.

Figure 2 shows that peak-to-peak spacing of a minimum of two pixels is required to be able to resolve two peaks and that thus the useable resolution of a spectrograph cannot be less than two detector pixels.² This means that in order to take full advantage of its 1000 spectral channel resolution, the Triplet Spectrograph is designed with a 2048 pixel detector.

With its novel optical design that supports high-resolution spectroscopy at a relatively short focal length, the Triplet Spectrograph is able to cover the spectral range from 50–3500 cm^{-1} at 4 cm^{-1} spectral resolution, and is able to capture the full spectrum in a single exposure.

The design contains no moving parts, which makes it easy to replace gratings to accommodate a range of excitation lasers and minimizes maintenance costs. The Triplet Spectrograph is also able to accept high-resolution gratings that deliver 2 cm^{-1} resolution over the range from 50–1800 cm^{-1} .

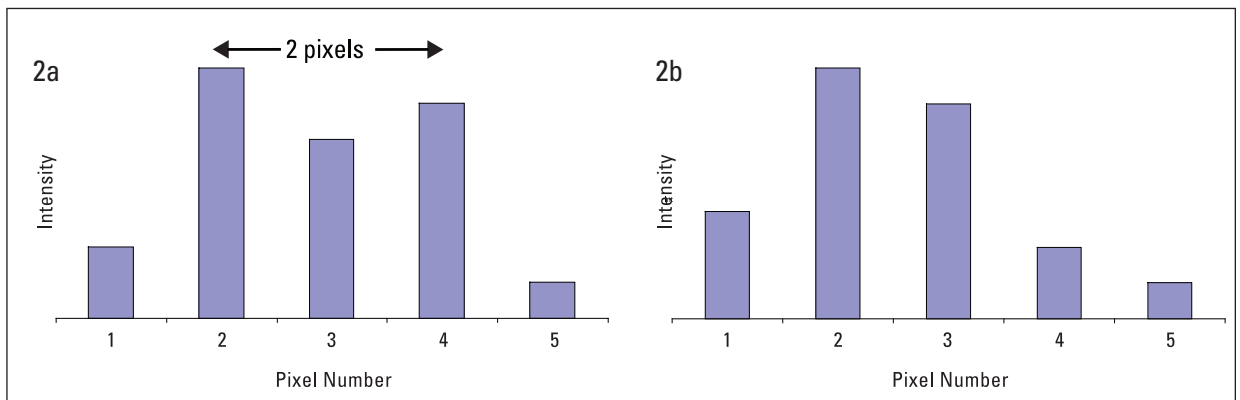


Figure 2: The effect of the number of pixels on resolution. In Figure 2(a) the two peaks at pixel numbers 2 and 4 are clearly resolved. In Figure 2(b) it is not possible to determine whether the peaks at pixels 2 and 3 are distinct from each other or are part of a single broad peak.

Performance Results

Figure 3 shows a neon emission spectrum collected on the Triplet Spectrograph. A close-up of three of the peaks shows the spectral quality of the spectrograph (Figure 4). Peak widths are approximately 2 pixels and are equal to the theoretical performance of the spectrograph. The peak shapes are excellent.

A grating spectrograph has a roughly constant resolution across its spectral range if the resolution is given in wavelength units. As a result, when the resolution of a spectrograph is measured on a wavenumber (cm^{-1}) scale, as is preferred for Raman spectroscopy, it varies across the spectral range. An approximate formula converts wavelength resolution into wavenumber resolution.³

$$\delta k = \frac{10^7 \delta \lambda}{\lambda^2}$$

where:

δk = Wavenumber resolution in cm^{-1}

$\delta \lambda$ = Wavelength resolution in nm

Using the Gaussian best-fit data for the 22 most intense peaks in Figure 3, resolution in cm^{-1} is plotted against a fitting curve based on the theoretical resolution formula for a wavelength resolution of 0.19 nm. The results are shown in Figure 5. The DXR spectrometers also accept high-resolution gratings for measurements over the Raman spectral range of 50–1800 cm^{-1} . A plot using Gaussian best-fit data for the 11 most intense neon peaks collected using the high-resolution 633 nm grating is also shown in Figure 5. The curve is fit to a wavelength resolution of 0.09 nm.

For both gratings the fit is excellent. The resolution is better than 4 cm^{-1} in the middle of the full-range spectrum. The nominal resolution for the high-resolution grating is approximately 2 cm^{-1} .

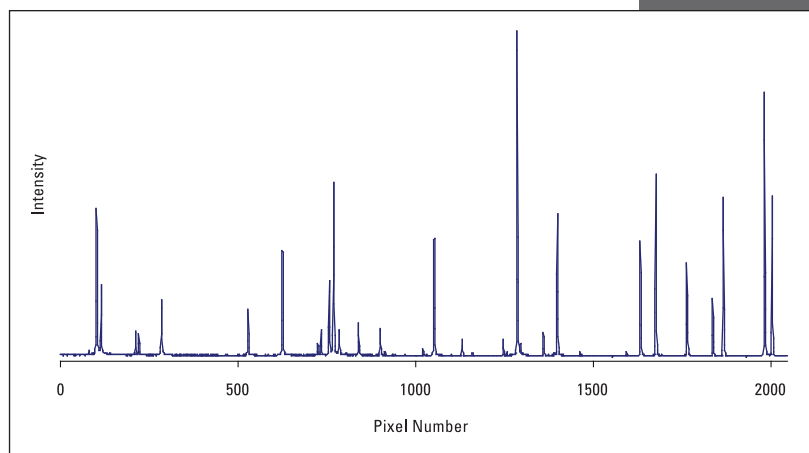


Figure 3: Neon emission spectrum collected using a Triplet Spectrograph with a full-range 633 nm grating and 25 μm entrance aperture. The neon emission lamp in the DXR calibration and alignment tool was used as the source.

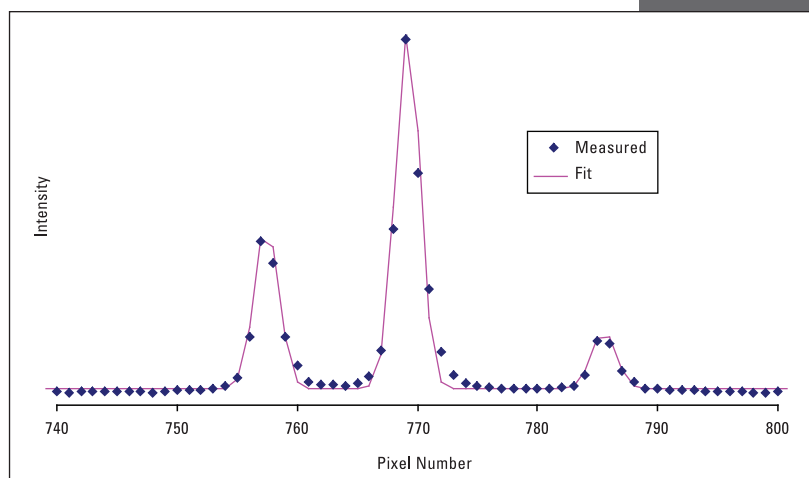


Figure 4: Close-up of neon emission peaks at approximately 757, 769 and 785 pixels. All three peaks are fit to Gaussian functions. Data collection conditions same as in Figure 3.

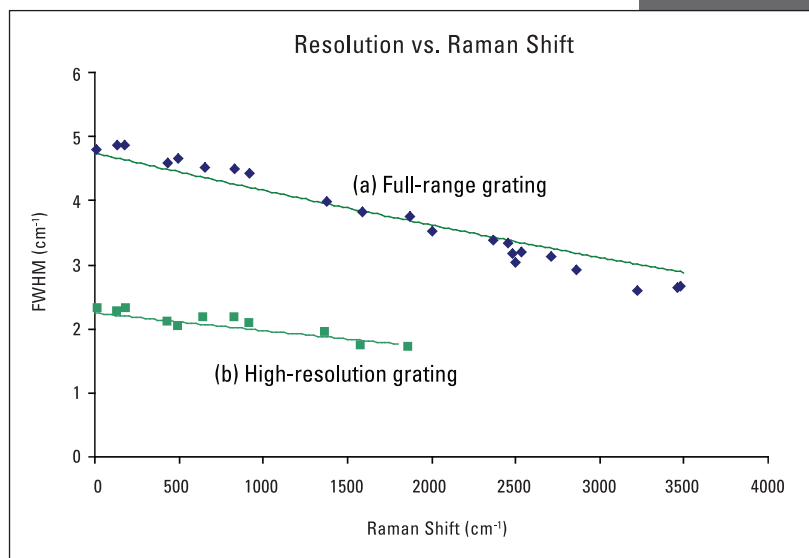


Figure 5: Plot of resolution vs. Raman shift, (a) for the 22 most intense neon emission peaks measured on the Triplet Spectrograph using the full-range 633 nm grating, (b) for the 11 most intense neon emission peaks measured using the high-resolution 633 nm grating. All data collected using a 25 μm entrance aperture. The neon emission lamp in the DXR calibration and alignment tool was used as the source.

Conclusion

The Triplet Spectrograph incorporates a 2048 pixel CCD detector and a novel optical design that supports high-resolution spectroscopy at a relatively short focal length. The spectrograph provides the performance required for routine yet rigorous analytical use. It captures a full spectrum from 50 to 3500 cm^{-1} in one exposure at a spectral resolution of 4 cm^{-1} . Unlike conventional designs, the Triplet Spectrograph provides optimal resolution and focus at all excitation wavelengths without compromise. In addition, it supports 2 cm^{-1} spectra over the fingerprint region from 50 to 1800 cm^{-1} . With no moving parts, it is a robust design that is low maintenance and supports multiple excitation lasers with the use of manually exchangeable gratings.

Footnotes

1. Patent pending.
2. Note that sometimes the *dispersion* of a spectrograph is specified, for example as units of cm^{-1} per pixel. The two-pixel rule suggests that the best possible spectral *resolution* is twice the dispersion value. In practice, it is probably greater than this, since the dispersion value does not account for a finite aperture width nor for any optical aberrations.
3. For this reason it is important when comparing spectrographs to note the wavenumber at which the spectral resolution has been measured. Resolution will always appear to be better at higher shifted wavenumbers.

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