TruRes - True resolution enhancement for optical spectroscopy

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Abstract

Resolving spectrally adjacent peaks is important for techniques, such as tracking small shifts in Raman or fluorescence spectra, quantifying pharmaceutical polymorph ratios, or molecular orientation studies. Thus, suitable spectral resolution is a vital consideration when designing most spectroscopic systems. Most parameters that influence spectral resolution are fixed for a given system (spectrometer length, grating groove density, excitation source, CCD pixel size, etc.). Inflexible systems are non-problematic if the spectrometer is dedicated for a single purpose; however, these specifications cannot be optimized for different applications with wider range resolution requirements.

Data processing techniques, including peak fitting, partial least squares, or principal component analysis, are typically used to achieve sub-optical resolution information. These techniques can be plagued by spectral artifacts introduced by post-processing as well as the subjective implementation of statistical parameters. TruRes™, from Andor Technology, uses an innovative optical means to greatly improve and expand the range of spectral resolutions accessible on a single setup. True spectral resolution enhancement of >30% is achieved without mathematical spectral alteration, data-processing, or spectrometer component changes. Discreet characteristic spectral lines from Laser-Induced Breakdown Spectroscopy (LIBS) and atomic calibration sources are now fully resolved from spectrally-adjacent peaks under otherwise identical configuration.

TruRes™ has added advantage of increasing the spectral resolution without sacrificing bandpass. Using TruRes™ the Kymera 328i resolution can approach that of a 500 mm focal spectrometer. Furthermore, the bandpass of a 500 mm spectrograph with would be 50% narrower than the Kymera 328i with all other spectrometer components constant. However, the Kymera 328i with TruRes™ is able to preserve a 50% wider bandpass.

Keywords: optical spectroscopy, resolution enhancement, LIBS, Raman, hyperspectral imaging, CCD, throughput

Introduction

Spectroscopic interrogation has become common place in both fundamental research and in applied sciences. Applications ranging from chemical detection, new material characterization, process instrumentation, and disease detection have employed spectroscopic characterization as their mode of operation. The two fundamental parameters that characterize a spectroscopy instrument are bandpass and resolution, or the size of the frequency space that can be interrogated simultaneously and the finite size that a delta function produces on the instrument respectively. These two are often coarsely inversely related, meaning bandpass generally decreases as the resolution increases and vice versa. Larger bandpass is important for characterizing a wide variety of phenomena simultaneously, while resolution is most crucial in elucidating low level information from a spectroscopic technique. For example, a high resolution IR spectrum of a gas phase molecule can resolve individual ro-vibrational modes and provide information regarding isotopic content of the sample.[1] In another example, high resolution Raman spectrum can provide more detailed characteristic peaks to aid in distinguishing two substances with similar vibrational signatures.[2] In the technique of Laser Induced Breakdown Spectroscopy (LIBS), simultaneous high resolution and large bandpass are required to adequately separate atomic spectral peaks over a broad spectral region, thus maximizing the number of peaks that can be identified.[3]

The resolution of a spectrograph is the product of several influencing parameters, including grating line density, entrance slit size, spectrometer optics, spectrometer focal length, and detector pixel pitch. Many of these parameters are fixed to a particular system configuration. For example, resolution can be improved by increasing the focal length of the spectrograph, but this requires significant alteration and realignment to the spectrograph optics or replacing the spectrograph entirely. Conversely, bandpass can be increased by using a lower groove density grating. Changing gratings has become much simpler over time with the addition of motorized multiple gratings turrets, but each grating is restricted to a single bandpass and resolution combination under otherwise unchanged system conditions. In these scenarios, the utility of a method of simultaneously increasing resolution and bandpass without the need to alter the spectrograph's optics becomes clear. In this work, we introduce TruRes™, an implementation of real-time resolution enhancement available on the Andor Kymera 328i spectrograph.

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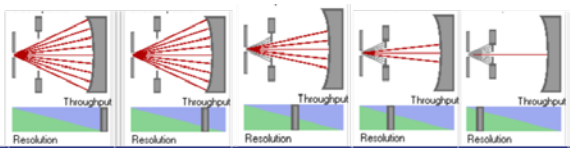
Methods of post hoc resolution enhancements involve post processing techniques, such as deconvolution, peak fitting or principal component analysis. Each of these techniques involves assumptions on the data and system response to interpolate data at higher resolutions. In many cases, this can lead to unwanted artifacts that result in increased or less information than previously existed (fig. 3). TruRes™ uses an innovative optical means to produce a true spectral resolution enhancement without mathematical spectral alteration, data-processing or spectrometer component changes, to greatly improve and expand the range of spectral resolutions accessible on a single spectrograph configuration. This increases the versatility of the spectrometer and allows one to fine tune the spectral resolution without sacrificing spectral bandpass. The performance of TruRes™ is characterized by use of a neon calibration source and actual LIBS spectral data. TruRes™ enhancement shows an increase of resolution by >30%, approaching the resolution level of a 500 mm spectrometer, while maintaining the bandpass of a 328mm spectrometer. In addition to the spectral resolution improvement in the horizonal plane, better spatial separation is also observed in the vertical imaging plane of the TruRes™ enhanced spectrograph. Two-dimensional enhancement allows imaging of greater hyperspectral track densities with tunable resolution across the entire length of the sensor.

Experimental

TruRes™ was characterized on a Kymera 328i imaging Czerny-Turner spectrograph (Andor Technology, Belfast, UK). The spectrograph was configured with a 300 grooves/mm plane reflectance grating blazed at 500 nm (Richardson, UK). The Kymera 328i was equipped with a toroidal collimating mirror to correct for astigmatic aberration and produce a 328 mm focal length. Light was coupled into the spectrometer via a 19-channel multimode fiber bundle (100 um cores, NA 0.22) which terminated in a ferrule containing a linear fiber stack positioned at the entrance slit (50 μm) of the spectrometer. A Newton 920 spectroscopic CCD camera with a pixel resolution of 1024 x 255 and pixel pitch of 26 μm was coupled to the direct output port of the Kymera 328i (Andor Technology, UK). Spectral samples consisted of light from a Neon calibration lamp (Ocean Optics, St. Petersburg, Florida) and atomic emission from a steal sample produced via LIBS.

Results and discussion

Hyperspectral imaging requires an imaging grade spectrograph in order to sufficiently separate and characterize each spectral signature. Point sources imaged through a spectrograph generally suffer from off axis aberrations such as coma, oblique astigmatism, and spherical aberration[4]. These result in out-of-focus and asymmetric blur patterns of the point source imaged onto the detector. This can be mitigated by careful optical correction introduced in the collimating mirror, such as the toroidal mirrors used in imaging spectrographs. Despite this correction, image reproduction remains non-ideal for Czerny-Turner spectrographs (fig. 2). Longer focal length spectrographs suffer less from these aberrations due to their increased operating F#. Higher F# light has a narrower divergence cone and consequently shallower off axis rays.



Iris position	100	80	50	30	10
F/#	4.1	4.3	6.5	10.8	32.5
NA	0.123	0.117	0.077	0.046	0.012
Cone angle (°)	14.1	13.4	8.8	5.3	1.4
Solid angle	4.7×10^{-2}	4.3×10^{-2}	1.9×10^{-2}	6.7×10^{-3}	4.5×10^{-4}
Peak area	100%	90%	39%	14%	1%

Figure 1. Representation of the mechanism of the TruRes™ iris. The iris is placed behind the input slit where input light is diverging. Closing the iris blocks oblique angle rays increasing the effective f/# of the input light. Iris diameter is calibrated to represent % open. The table below correlates iris position to effective f/#, numerical aperture, cone angle, solid angle and peak area % with 100% open equaling F/4.1.

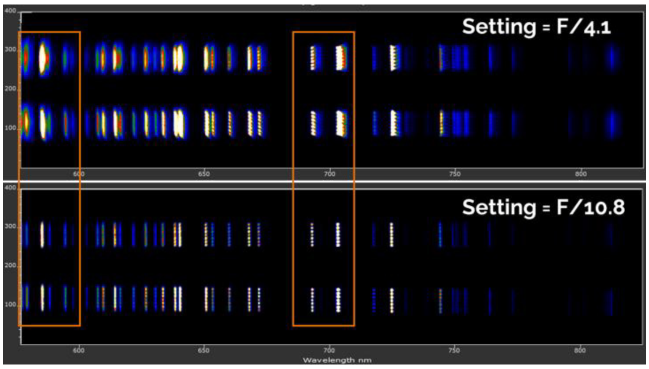


Figure 2. Comparison of 1st order diffracted image of lines from a neon calibration source coupled through 100 um core fiber stack at f/4.1 (100% iris) and f/10.8 (30% iris). Substantial improvement in image sharpness is seen at higher f/#'s.

TruRes™ resolution enhancement technique utilizes a motorized iris strategically placed along the optical path on the interior of the input slit, essentially spatially filtering naturally diverging light through the slit.

High angle rays, which lead to aberrations, are blocked as the iris is closed, which effectively increases the input f/#. An illustration of the varying calibrated iris positions and their effect on input f/# and spectral peak area can be found in figure 1. This, in effect, is mimicking the optical characteristics of a longer focal length spectrograph, resulting in improved point source image reproduction and minimizing blurry or asymmetric imaging of the fiber bundle. A comparison of the imaging performance of the fully opened aperture (f/4.1) with the iris closed to 30% (f/10.8) is shown in figure 2.

When full vertically binned, increased imaging performance from mitigating aberrations results in an increased spectral resolution as demonstrated in figure 3. Here we see the 753.577 and 754.404 nm go from an unresolved doublet with the iris fully open (F/4.1) to two fully resolved peaks with the iris at 50% (F/6.5). By contrast, a standard mathematical resolution enhancements that fits gaussian instrument response functions to peaks failed to resolve the individual peaks in the neon doublet.

Throughput decrease is a consequence of the iris closing; however, it is important to note that the relationship between iris position and spectral peak height is far from linear. A significant amount of throughput sacrificed is from the aberration-filled outer edges of the input beam, resulting in a much smaller impact on peak intensity than one may expect. Firstly, for the majority of 1/3 meter spectrographs (including the Kymera 328i), a point source such as a fiber at the input focal plane propagating at f/4.1 will diverge such that its collimated area will overfill the grating. Thus, increasing from f/4.1 to f/5.1 results in almost no appreciable throughput loss (illustrated in figure 4). Furthermore, throughput will continue to decrease sigmoidally, not linearly, with smaller throughput losses at wider iris positions if a Gaussian distribution intensity is assumed (figure 5).

As the iris closes, f/# increases and imaging performance improves in both spatial planes. The resolution increase is characterized with the 546-nm line of a mercury-argon calibration source coupled to a 10 µm entrance slit of the Kymera 328i. The spectrograph was equipped with a 1200 l/mm grating and a Newton 920 CCD detector (figure 6). Relative improvement in resolution is observed as throughput (measured by spectral peak intensity) decreases until very small iris diameters are reached.

The increase in resolution was also characterized for several mercury-argon lines spanning the UV-Vis spectrum. Relative resolution improvement is largely independent of specific spectral region (UV to Vis to NIR). It is also evident that the iris position where the FWHM is minimized is not the smallest iris aperture. Instead, the minimum occurs at 20-30% of fully open, after which the FWHM trend seems to level off (Figure 7). This may be due to reaching a crossover point in which the resolution gained from mitigating aberrations is now counteracted by a resolution loss due to illuminating fewer and fewer grooves in the grating[5].

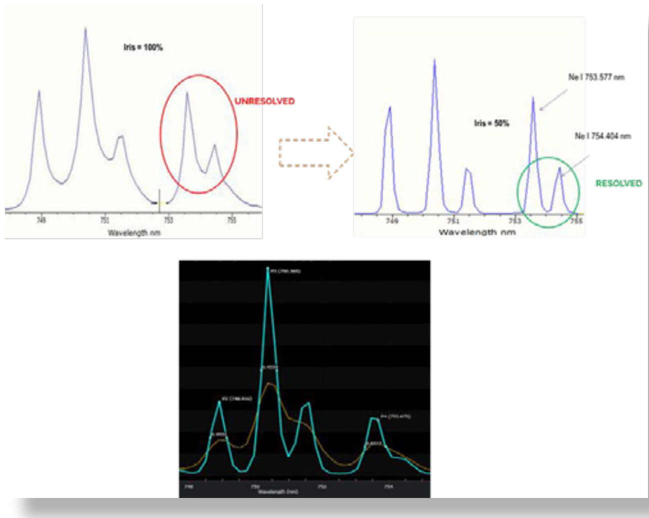


Figure 3. TruRes™ resolution improvement on 753 and 754 lines of Ne 1(top) compared with mathematical peak fitting algorithm (bottom).

Finally, a case study employing a LIBS characterization of a steel sample was conducted. We can see that applying the TruRes™ aberration correction allows for the resolving of extra structure in the spectra that previously appear as peak shoulders (~275 nm) or in some cases components that were completely buried in their adjacent peak (286.8 nm and 287.1 nm). This added information is useful for perhaps identifying trace components in the steel sample were being missed, or in providing and extra criterion for mitigating false positive and negative error rates in identification algorithms. From the comparison is it also evident that the throughput has decreased significantly, however for high light level techniques this is less of a problem as evidenced by the continued high signal-to-noise ratio in the resolution enhanced spectrum (figure 8).

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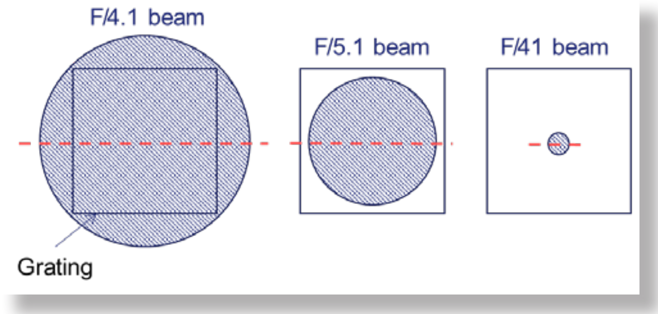

Figure 4. Effect of increasing F/# to assure the grating is not overfilled.

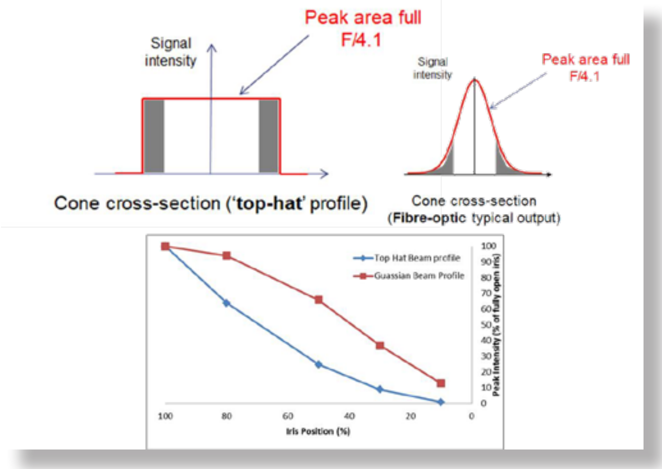

Figure 5. Comparison of effect of beam intensity profile on throughput decrease during iris closure sequence.

It is also important to note that bandpass of the measurement did not change despite the increase in resolution. This is particularly important in LIBS applications as atomic emission lines can span a large amount of wavelength space (~500 nm) and thus maintaining a bandpass that covers the maximal wavelength space is essential.

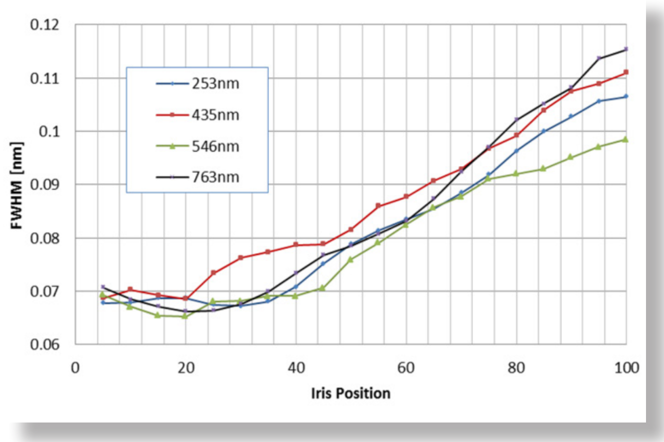

Figure 7. FWHM is shown as a function of iris position for 4 mercury-argon lines across different parts of the UV-Vis-NIR spectrum.

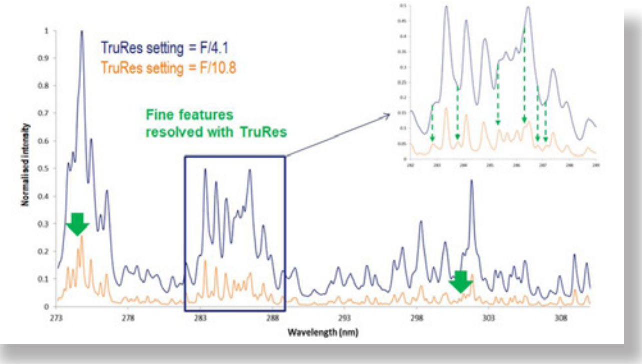

Figure 8. LIBS spectrum of steel TruRes™ iris positions of 100% and 30% corresponding to F/4.1 and F/10.8 respectively. Resolution improvement shows extra resolved structure called out by green arrows. Data is courtesy of Dr. Vincent Motto-Ros, Institut Lumiere Matiere (ILM), Lyon University.

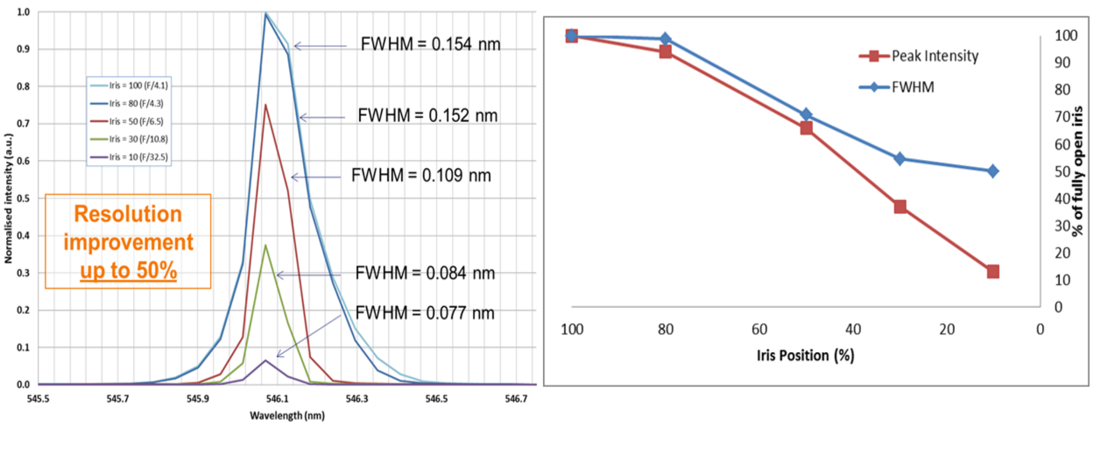

Figure 6.
546-nm peak of mercury-argon line calibration source at varying iris positions (left).

The decrease in throughput in conjunction with an increase in resolution can be seen (right).

TruRes - True resolution enhancement for optical spectroscopy

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Conclusion

Here we have characterized the capabilities of the TruRes™ resolution enhancement mechanism found on the Andor Kymera 328i imaging spectrograph. We have shown that the novel implementation of an iris behind the input slit can be used to manipulate the input f/# of the spectrograph, blocking oblique rays which cause spherical aberrations resulting in a higher resolution measurement by up to 50%. This can be accomplished without changing the grating or spectrometer focal length, which preserves the wider bandpass of a shorter focal length spectrometer or lower line density grating. For comparison, with the iris optimally closed the Kymera 328i has a measured FWHM of ~0.08 nm with a 1200 l/mm grating, while a 500 mm focal length spectrometer would be expected to have a ~0.07 nm FWHM with an equivalent grating. Thus, the Kymera 328i resolution can approach that of a 500 mm focal spectrometer. Furthermore the bandpass of a 500 mm spectrograph with would be ~38 nm while the Kymera 328i would preserve its 50% wider band pass of 58 nm. While this results in a relatively small reduction in signal throughout, for many higher photon flux applications, throughput can often be sacrificed in favor of resolution that can aid in identification and differentiation of chemical species.

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