Dispersive Raman Imaging

- Review of Spectrograph Designs and the Impact on Spectral & Spatial Resolution -

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Abstract

Raman spectroscopy is experiencing a rapid increase in commercial and military application integration. There has been a large amount of commercial discussion regarding relatively low cost, low resolution single point (single fiber) spectrometers for handheld transportable applications, although only limited advancement of higher performance designs. Applications which require maximum signal collection and dynamic range, including those which require multi-channel or other input aperture imaging capability will benefit if one can fill the entire height of the tallest spectroscopy CCD with minimal distortion of the input image.

Most commercially available dispersive spectrometer optical designs have difficulty imaging all field points of the full Raman spectral bandwidth onto a flat focal plane simultaneously. Czerny-Turner designs are typically throughput limited to approximately f/4 or slower, and exhibit relatively high image distortions as one moves further away from the central input axis (spatially over the slit height) as well as along the spectral axis. Torroidal mirrors are often employed to minimize this effect, although this provides optimized correction for only one point on the focal plane. Others, which are based on axial-transmissive designs, suffer at short focal lengths from chromatic aberrations, smile, and keystone. For best results, these often require the use of curved input apertures, non-standard refractive lens material selection, and wavelength optimized anti-reflective coatings on each lens surface to compensate for chromatic aberrations, reflection losses, and potential ghost images. In addition, common axial-transmissive designs suffer from throughput vignetting at both the short and long wavelength regions.

This paper describes the performance of Headwalls' Raman Explorer™, a novel aberration corrected high reciprocal dispersion retro-reflective concentric imaging spectrograph design with multiple inputs and high efficiency through resonance, which produces minimal image blur over the full CCD focal plane with exceptionally high signal to noise efficiency and f/2.4 throughput. This design images 1:1 straight slit or stacked linear arrays of optical fibers covering the full height of spectroscopy CCD's with optimal channel separation and no image curvature.

Objective

Any degradation of an image which is launched into a spectrograph, whether it's a single fiber core, a large stack of multiple fibers, or an input slit will impact its' spectral resolving power, optical throughput efficiency, and multi-channel crosstalk performance. The quality of both spectral and spatial input image reproduction at the spectrograph exit focal plane is an often overlooked parameter when optimizing spectrometer designs.

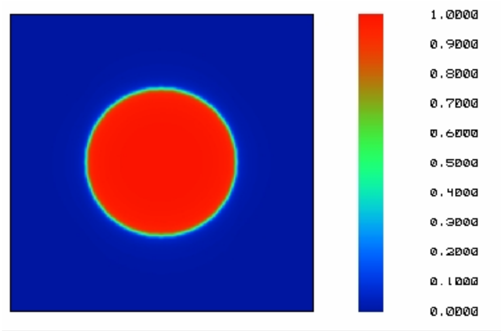


Image A: Theoretical / modeled

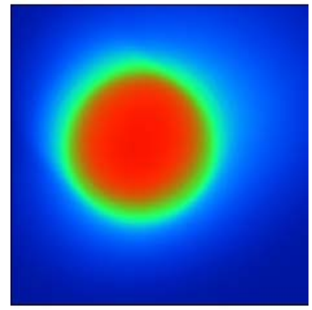


Image B: Desired spatial image resolution at all spectral and spatial points on the focal plane

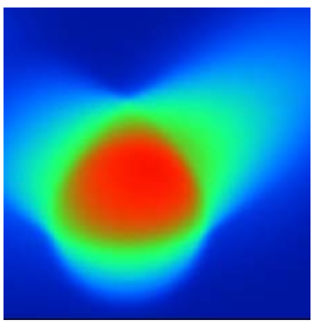


Image C: Example of distortion

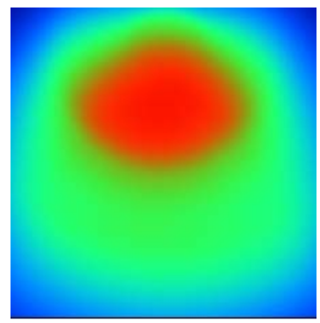


Image D: Example of distortion

Figure 1

The ray trace images shown in Figure 1 provide examples of nominal spectral image distortion. Image A represents a theoretical 50 µm dia. image of uniform intensity at a specific wavelength. At varoius spatial positions over a focal plane, one would like to maintain this shape, or the shape observed in Image B as well as possible. Although, if a spectrograph design perscription is not optimized, aberrations distort the size and shape of the spectral image causing rays intended for that wavelength and spatial position to fall on adjacent locations, thereby corrupting the spectral purity of the measured results. Images C and D provide examples of emerging image distortions, and are minimal in relation to the extent they can degrade in commonly accepted "Research Grade" spectrograph designs. As the data we collected demonstrates, the Raman Explorer does an exceptional job at maintaining high spatial and spectral integrity similar to Image B over the entire focal plane.

This study evaluated the spectral and spatial imaging performance of the patented Raman Explorer™, a family of aberration corrected high reciprocal dispersion retro-reflective concentric imaging spectrographs which produce minimal spot blur over the full CCD focal plane. The objective of this evaluation was to obtain spectral intensity data which can be interrogated to display:

1. Image shape.
2. A comparison of FWHM spectral and spatial resolution resulting from 50 µm diameter fiber cores with and without a 10 µm slit aperture.
3. Quality of horizontal and vertical image maintenance (keystone and smile distortion eliminated).

Examples of Typical Design Distortions

Axial Transmissive

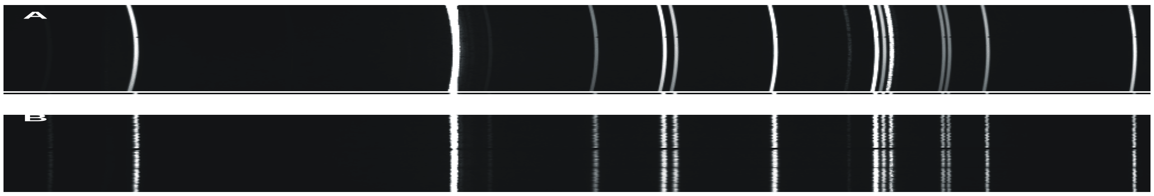


Figure 2 *Z. Huang, H. Zeng et al, Optics Letters, 26, 1782-1784, 2001*

The top image in Figure 2 shows the resulting curvature of a straight line entrance slit through an Axial Transmissive Kaiser Holospec™ spectrograph. The entrance slit was illuminated by an atomic emission source. This is a well understood result of short focal length high numerical aperture spectrograph designs which employ plane gratings. An aberration such as this decreases spectral resolving power, potential signal to noise performance, and creates a challenge with wavelength calibration.

Many integrators of this type of spectrograph design restrict the input image height to compensate for this performance issue, resulting in sacrificed signal capture. Others, as demonstrated in the lower image in Figure 2 have compensated for this aberration by laser drilling a custom entrance aperture in the reverse orientation of the horizontal parabolic shaped aberrated displacement.

Czerny-Turner

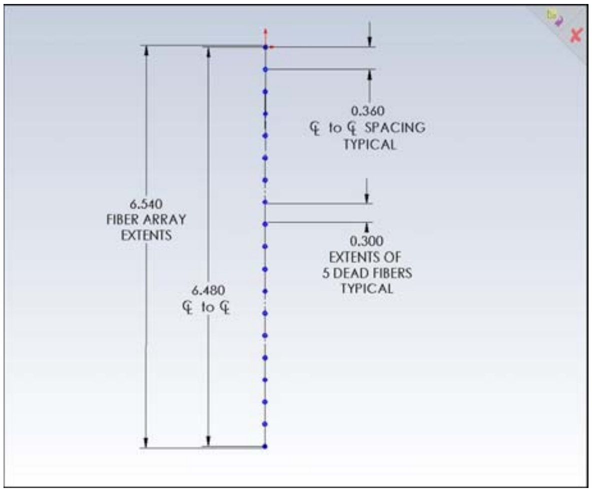
Figure 3

Figure 3 shows an image taken from a 150mm focal length Czerny-Turner imaging spectrograph which used a torroidal mirror for image correction. Spectral bandwidth is approximately 2000 cm-1 from a 532 nm laser. Two adjacent 50µm fibers which are separated by the combined 20µm of cladding and buffer layer were isolated within an array. Note the spatial broadening of the images as wavelength increases left to right. This broadening will cause inaccurate fractional ray blur on adjacent pixels in both the spectral and spatial domains, and contaminate spectral and optical throughput purity.

Raman Explorer™ Spectral and Spatial Resolution Evaluation

We have performed an evaluation of fine spectral and spatial imaging resolution capabilities and signal throughput characteristics of our Raman Explorer 785 f/2.4 spectrograph over the area of an Andor Newton camera which included a 2048 x 512 array that has 13.5 micron square pixels. The following is a summary of these results.

To enable imaging of narrow spectral lines, we aligned a test fiber assembly to the channel 1 entrance aperture of a Raman Explorer 785 imaging spectrometer. As shown in Figure 4, the test fiber assembly is configured of an array of 19 live 50/60/70 um fibers each separated by 5 dead fibers.



Raman Explorer™

Large area precision focal plane

Figure 4

This fiber assembly allows us to place live 50 um core fiber images over 6.5 mm of the available 7 mm of entrance aperture height at 360 um center to center distances. Using Neon and Argon atomic line sources to illuminate spectral lines across the full spectral bandwidth of the CCD, our engineers used the following method to capture meaningful spatial and spectral data points:

1. Focused the fiber images and adjusted the light source intensity and camera integration time to just reach, but stay within saturation limits of brightest line. We then set integration time so that readout smear between channels was minimized, set background subtraction, and captured and stored the image.
2. Same conditions as above, except placing a 10 micron slit over the ferrule face. Take and store image.

This illumination provides narrow band spectral images of each fiber aperture over the complete focal plane, and enables interrogation of the extreme spatial and spectral imaging capabilities of this spectrometer. As displayed in Figure 5, horizontal and vertical positions are held within 1 pixel deviation.

In order to provide a baseline illumination for comparison of throughput vs. integration time, an argon pen lamp was inserted into a holder and adjusted so that the 794.82 nm line saturated a pixel within any of the available fiber input/image channels in approximately 0.80 sec. The lamp was then secured in this position.

Pixel A/D counts were summed in spatial and spectral direction for each fiber image under test. The SUM is divided by the MAX SUM and multiplied by 2^16 (16 bit) to simulate an integration time which just reached the saturation point of the register in a binning application. The pixel A/D count of each fiber image under test was divided by the maximum A/D count within that image and shown in a scale from 0.0 to 1.0 and color coded to depict image performance. The spatial and spectral imaging resolution was plotted and the FHWM is measured from the plots and reported.

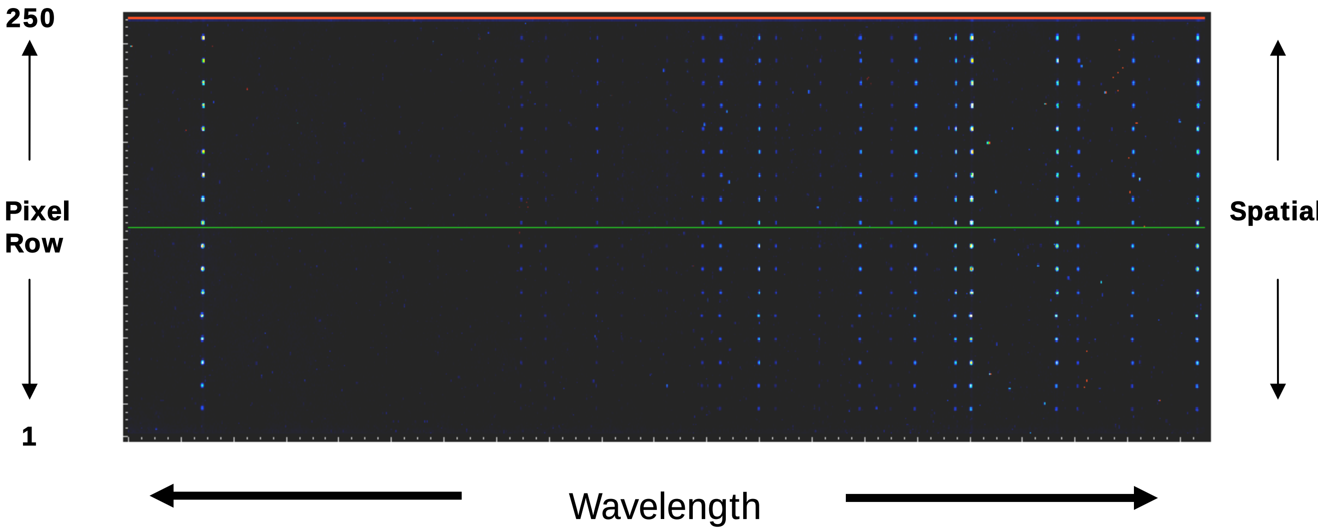


Figure 5

Figure 5 shows the spectral images produced by Neon and Argon illumination through a Raman Explorer. Fiber is 50 µm dia., and pixel size is 24 µm square. Horizontal, vertical, and FWHM imaging was pixel limited.

Results for the full 50 um fiber images, and 50 um fiber with 10 um slit images are shown in Tables 1A, 1B, and 2. The color coded pixel maps display the individual pixels' relative intensity and spatial area which covers >/= 50% (FWHM) of the hottest pixel value at near saturation level for that wavelength at three spatial and wavelength extremes. Reminder, the pixels are 13.5 um square, the fiber is 50 um core with a 10 um cladding, and as you will see in all cases the images are maintained with superb accuracy.

Table 2 illustrates that a Raman Explorer designed for 785 nm laser stimulation, and integrating a CCD with a 13.5 µm pixel pitch and 10 µm wide entrance aperture is capable of 3.7 cm-1 spectral resolution over the fingerprint region, and 2.6 cm-1 over the CH stretch region.

Headwall PHOTONICS

PIXEL COLORING LEGEND	
GREEN	50—70% of peak
YELLOW	70—90% of peak
RED	90—100% of peak

Table 1

T1, 5185-7312, Fiber Optic Cable Array, Reformatter 6.54, 50 um fiber core, 60 um diam clad

Wavelength = 794.82 nm

Resolution (FWHM)				
	Spectral		Spatial	
Fiber	Pix	cm-1	Pix	um
1	3.7	5.7	4.5	60.8
10	3.5	5.3	3.6	48.6
19	4.3	6.6	4.5	60.8

Fiber 1

0.16	0.44	0.64	0.65	0.36	0.08
0.23	0.67	0.94	0.93	0.55	0.17
0.25	0.72	1.00	0.98	0.59	0.22
0.19	0.58	0.89	0.90	0.54	0.19
0.12	0.34	0.52	0.52	0.32	0.13
0.08	0.21	0.28	0.24	0.15	0.07

Fiber 10

0.09	0.32	0.48	0.34	0.17	0.07
0.25	0.66	0.91	0.78	0.43	0.16
0.33	0.76	1.00	0.99	0.60	0.19
0.23	0.62	0.86	0.78	0.44	0.15
0.08	0.28	0.44	0.34	0.18	0.07
0.02	0.08	0.13	0.12	0.06	0.02

Fiber 19

0.27	0.38	0.41	0.31	0.17	0.08
0.39	0.62	0.73	0.57	0.34	0.13
0.49	0.85	1.00	0.80	0.49	0.17
0.51	0.86	0.99	0.80	0.51	0.16
0.38	0.63	0.73	0.62	0.37	0.11
0.23	0.33	0.36	0.29	0.16	0.04

Wavelength = 842.46 nm

Resolution (FWHM)				
	Spectral		Spatial	
Fiber	Pix	cm-1	Pix	um
1	5.0	6.8	4.8	64.8
10	3.5	4.8	3.6	48.6
19	3.5	4.8	3.6	48.6

Fiber 1

0.28	0.49	0.70	0.74	0.63	0.47
0.33	0.58	0.83	1.00	0.94	0.66
0.34	0.61	0.83	0.97	0.94	0.65
0.31	0.53	0.69	0.74	0.70	0.55
0.26	0.41	0.49	0.44	0.31	0.22
0.20	0.30	0.32	0.25	0.14	0.07

Fiber 10

0.04	0.14	0.24	0.28	0.19	0.08
0.10	0.33	0.61	0.68	0.42	0.17
0.20	0.59	0.95	0.98	0.71	0.33
0.22	0.62	0.94	1.00	0.75	0.41
0.15	0.40	0.67	0.77	0.54	0.21
0.07	0.15	0.25	0.30	0.21	0.08

Fiber 19

0.05	0.18	0.23	0.17	0.11	0.05
0.15	0.48	0.56	0.43	0.19	0.05
0.33	0.75	0.88	0.77	0.29	0.05
0.39	0.83	1.00	0.91	0.34	0.07
0.25	0.70	0.89	0.76	0.35	0.10
0.09	0.35	0.51	0.45	0.28	0.09

Wavelength = 965.78 nm

Resolution (FWHM)				
	Spectral		Spatial	
Fiber	Pix	cm-1	Pix	um
1	4.6	4.8	5.5	74.3
10	3.5	3.6	4.2	56.7
19	4.0	4.1	3.7	50.0

Fiber 1

0.29	0.49	0.65	0.60	0.45	0.25
0.36	0.63	0.86	0.88	0.65	0.34
0.37	0.71	1.00	1.00	0.72	0.35
0.33	0.62	0.89	0.95	0.74	0.40
0.26	0.45	0.62	0.65	0.48	0.26
0.21	0.32	0.38	0.36	0.25	0.14

Fiber 10

0.04	0.14	0.28	0.29	0.17	0.08
0.10	0.36	0.57	0.49	0.30	0.12
0.23	0.72	0.92	0.80	0.40	0.12
0.28	0.76	1.00	0.91	0.47	0.11
0.19	0.60	0.83	0.80	0.37	0.10
0.10	0.29	0.46	0.39	0.21	0.08

Fiber 19

0.16	0.20	0.25	0.22	0.13	0.06
0.33	0.59	0.70	0.57	0.30	0.13
0.50	0.91	1.00	0.80	0.54	0.20
0.50	0.92	0.96	0.80	0.50	0.14
0.33	0.56	0.62	0.47	0.20	0.05
0.14	0.17	0.17	0.11	0.05	0.02

Table 1A

Raman Explorer 785, 2048 x 512, 13um square pixels

5185-7312, Fiber Array, Reformatter 6.54, 50 um fiber core, 60 um dia clad

Wavelength = 794.32 nm					Wavelength = 842.46 nm					Wavelength = 965.78 nm				
Resolution (FWHM)					Resolution (FWHM)					Resolution (FWHM)				
	Spectral		Spatial			Spectral		Spatial			Spectral		Spatial	
Fiber	Pix	cm-1	Pix	um	Fiber	Pix	cm-1	Pix	um	Fiber	Pix	cm-1	Pix	um
[illegible]	3.7	6.7	4.5	60.8	1	5.0	6.8	4.8	64.8	1	4.6	4.8	5.5	74.3
10	3.5	6.3	3.3	48.6	10	3.5	4.8	3.6	48.6	10	3.5	3.6	4.2	56.7
19	4.3	6.6	4.5	60.8	19	3.5	4.8	3.6	48.6	19	4.0	4.1	3.7	50.0

Fiber 1

0.16	0.44	[illegible]	[illegible]	[illegible]	0.08
0.23	[illegible]	[illegible]	[illegible]	[illegible]	0.17
0.25	[illegible]	[illegible]	[illegible]	[illegible]	0.22
0.19	0.58	[illegible]	[illegible]	[illegible]	0.19
0.12	0.34	0.52	0.52	0.32	0.13
0.08	0.21	0.28	0.24	0.15	0.07

Fiber 1

0.28	0.46	[illegible]	[illegible]	[illegible]	0.47
0.33	0.58	[illegible]	[illegible]	[illegible]	[illegible]
0.34	0.61	[illegible]	[illegible]	[illegible]	[illegible]
0.31	0.53	[illegible]	[illegible]	[illegible]	0.55
0.26	0.41	0.49	0.44	0.31	0.22
0.20	0.30	0.32	0.25	0.14	0.07

Fiber 1

0.29	0.49	[illegible]	[illegible]	[illegible]	0.25
0.36	[illegible]	[illegible]	[illegible]	[illegible]	0.24
0.37	[illegible]	[illegible]	[illegible]	[illegible]	0.35
0.33	[illegible]	[illegible]	[illegible]	[illegible]	0.40
0.26	0.45	0.62	0.65	0.48	0.26
0.21	0.32	0.38	0.36	0.25	0.14

Fiber 10

0.09	0.32	[illegible]	[illegible]	0.17	0.07
0.25	[illegible]	[illegible]	[illegible]	[illegible]	0.16
0.33	[illegible]	[illegible]	[illegible]	[illegible]	0.19
0.23	[illegible]	[illegible]	[illegible]	[illegible]	0.15
0.08	0.28	0.44	0.34	0.18	0.07
0.02	0.08	0.13	0.12	0.06	0.02

Fiber 10

0.04	0.14	0.24	0.28	0.19	0.08
0.10	[illegible]	[illegible]	[illegible]	[illegible]	0.17
0.20	[illegible]	[illegible]	[illegible]	[illegible]	0.33
0.22	[illegible]	[illegible]	[illegible]	[illegible]	0.41
0.16	0.40	[illegible]	[illegible]	0.54	0.21
0.07	0.16	0.25	0.30	0.21	0.08

Fiber 10

0.04	0.14	0.28	0.29	0.17	0.08
0.10	[illegible]	[illegible]	[illegible]	[illegible]	0.12
0.23	[illegible]	[illegible]	[illegible]	[illegible]	0.12
0.28	[illegible]	[illegible]	[illegible]	[illegible]	0.11
0.19	0.60	[illegible]	[illegible]	0.37	0.10
0.10	0.28	0.46	0.38	0.21	0.08

Fiber 19

0.27	0.38	0.41	0.31	0.17	0.08
0.39	0.62	[illegible]	[illegible]	0.34	0.13
0.49	[illegible]	[illegible]	[illegible]	[illegible]	0.17
0.51	[illegible]	[illegible]	[illegible]	[illegible]	0.16
0.38	[illegible]	[illegible]	[illegible]	[illegible]	0.11
0.23	0.33	0.36	0.29	0.16	0.04

Fiber 19

0.06	0.16	0.23	0.17	0.11	0.06
0.16	[illegible]	[illegible]	[illegible]	0.19	0.05
0.33	[illegible]	[illegible]	[illegible]	[illegible]	0.05
0.30	[illegible]	[illegible]	[illegible]	[illegible]	0.07
0.26	[illegible]	[illegible]	[illegible]	0.35	0.10
0.09	0.36	0.61	0.45	0.28	0.09

Fiber 19

0.16	0.20	0.26	0.22	0.13	0.06
0.33	[illegible]	[illegible]	[illegible]	[illegible]	0.13
0.50	[illegible]	[illegible]	[illegible]	[illegible]	0.20
0.50	[illegible]	[illegible]	[illegible]	[illegible]	0.14
0.33	[illegible]	[illegible]	[illegible]	0.20	0.05
0.14	0.17	0.17	0.11	0.06	0.02

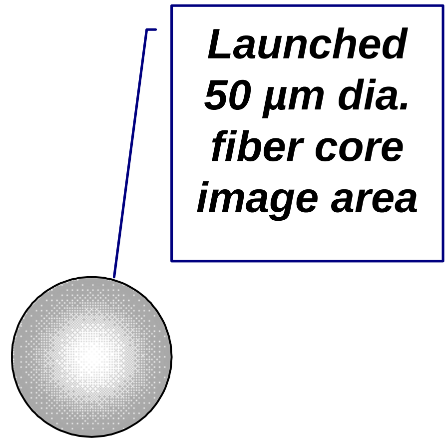


Table 1B

Table 2
T4, 5185-7312 Array with 10 um wide slit

Wavelength = 794.82 nm

Resolution (FWHM)

	Spectral		Spatial	
Fiber	Pix	cm-1	Pix	um
6	1.7	2.6	4.8	64.8
10	2.2	3.4	4.0	54.0
13	2.4	3.7	4.0	54.0

Fiber 6

0.00	0.02	0.16	0.53	0.26	0.04
0.00	0.03	0.38	0.95	0.29	0.04
0.01	0.03	0.41	1.00	0.24	0.03
0.00	0.03	0.39	0.89	0.18	0.02
0.00	0.02	0.27	0.60	0.14	0.02
0.00	0.01	0.06	0.16	0.06	0.01

Fiber 10

0.01	0.04	0.20	0.25	0.15	0.03
0.01	0.15	0.77	0.69	0.27	0.05
0.01	0.16	0.92	1.00	0.34	0.05
0.01	0.15	0.90	1.00	0.26	0.03
0.01	0.13	0.75	0.69	0.14	0.02
0.01	0.05	0.25	0.27	0.06	0.01

Fiber 13

0.01	0.09	0.38	0.40	0.19	0.03
0.01	0.18	0.76	0.96	0.34	0.05
0.02	0.22	0.90	1.00	0.36	0.05
0.02	0.27	0.91	0.96	0.29	0.04
0.01	0.19	0.60	0.55	0.14	0.02
0.01	0.05	0.18	0.13	0.04	0.01

Wavelength = 842.46 nm

Resolution (FWHM)

	Spectral		Spatial	
Fiber	Pix	cm-1	Pix	um
6	3.5	4.8	4.5	60.8
10	2.8	3.8	4.0	54.0
13	2.5	3.4	4.0	54.0

Fiber 6

0.07	0.27	0.41	0.36	0.18	0.05
0.15	0.45	0.70	0.68	0.41	0.14
0.24	0.63	0.99	1.00	0.62	0.25
0.29	0.66	0.96	0.88	0.52	0.21
0.23	0.53	0.79	0.70	0.44	0.18
0.13	0.31	0.46	0.38	0.29	0.19

Fiber 10

0.00	0.02	0.08	0.16	0.12	0.05
0.01	0.06	0.28	0.45	0.32	0.12
0.02	0.13	0.64	1.00	0.55	0.20
0.02	0.17	0.73	0.96	0.58	0.24
0.02	0.13	0.61	0.82	0.49	0.21
0.01	0.07	0.34	0.50	0.36	0.17

Fiber 13

0.01	0.03	0.13	0.22	0.13	0.04
0.01	0.10	0.55	0.72	0.28	0.07
0.02	0.13	0.73	1.00	0.44	0.12
0.02	0.12	0.67	0.92	0.47	0.16
0.01	0.09	0.59	0.75	0.40	0.16
0.01	0.03	0.17	0.28	0.26	0.12

Wavelength = 965.78 nm

Resolution (FWHM)

	Spectral		Spatial	
Fiber	Pix	cm-1	Pix	um
6	2.1	2.2	5.0	67.5
10	2.2	2.3	4.7	63.5
13	2.2	2.3	4.6	62.1

Fiber 6

0.03	0.09	0.31	0.62	0.41	0.13
0.04	0.14	0.43	0.98	0.59	0.18
0.05	0.18	0.46	1.00	0.50	0.15
0.05	0.18	0.43	0.93	0.43	0.13
0.04	0.14	0.31	0.66	0.32	0.12
0.02	0.08	0.16	0.26	0.11	0.04

Fiber 10

0.01	0.05	0.23	0.53	0.30	0.06
0.02	0.09	0.68	0.88	0.30	0.06
0.03	0.13	0.84	1.00	0.27	0.05
0.03	0.15	0.85	0.92	0.20	0.04
0.03	0.13	0.78	0.75	0.15	0.04
0.02	0.07	0.30	0.36	0.12	0.03

Fiber 13

0.01	0.02	0.08	0.26	0.18	0.04
0.02	0.06	0.36	0.62	0.29	0.06
0.02	0.11	0.84	0.95	0.33	0.07
0.03	0.13	0.89	1.00	0.28	0.05
0.02	0.14	0.94	0.81	0.17	0.04
0.02	0.10	0.60	0.48	0.10	0.02

Table 2

Summary

The spectral and spatial imaging properties of a spectrograph play an important role in the ability of a spectrometer to produce spectrally pure results.

The spectral and spatial imaging performance of the patented Raman Explorer™ aberration corrected high reciprocal dispersion retro-reflective concentric imaging spectrographs produce minimal image blur, and no smile or keystone over the full CCD focal plane. This performance is superior to traditional Czerny-Turner and axial-transmissive designs, and enables higher signal levels, lower optical noise, as well as high spectral resolution over the full Raman bandwidth. This design is optimized for processing large numbers of collection fibers individually or simultaneously.

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