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High-Efficiency Diffuse Raman Spectroscopy Through a Fiber Bundle

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Abstract— **Conventional spectrometers are limited in the amount of light they accept because of the requirement for narrow input apertures. A trade-off must generally be made between spectral resolution and input aperture width. This is especially a problem for performing spectroscopy on diffuse sources, such as with tissue, from which signal light has a broad spatial distribution. We introduce a method for achieving good spectral resolution from a fiber bundle input. The image of a fiber bundle has a characteristic structure. By distorting this image optically, we generate a pseudo-orthogonal intensity mask at the input of the spectrometer. The pseudo-orthogonal properties of the mask then allow decoupling at the detector plane of wavelength from spatial position. As long as the distorted image of the fiber bundle is well known, a spectrum can be recovered with spectral resolution equivalent to that of a conventional slit-based spectrometer. We demonstrate successful recovery of narrowly spaced spectral features as well as Raman spectra from a highly scattering sample with this method. This method enables probes with much higher throughputs and add fiber bundle-based spectroscopy to endoscopic designs.**

I. Introduction

Fiber bundle collection is a popular and desirable way to perform tissue spectroscopy, either through endoscopes or simple probes. This is because optical fibers are flexible and easy to place against tissue in difficult to reach regions (endoscopes). Each fiber is limited in the amount of light it collects from a diffuse sample such as tissue, and so large bundles of fiber can increase collected light by up to several order of magnitude. However, there are significant barriers to using light from a fiber bundle for high resolution spectroscopy.

When one performs tissue spectroscopy, especially Raman spectroscopy, the measurements are most often limited by the low quantities of light collected. Conventional spectrometers require a narrow spatial distribution of light to achieve acceptable spectral resolution, which is most often accomplished by collecting light with a narrow slit or single fiber. A narrow input aperture can seriously reduce the amount of light which is captured by the spectrometer for many applications. Light collected from biological samples, for example, is often diffuse and distributed among many optical modes which are impossible to simultaneously focus to the same position. If one wishes to collect more light from a diffusely radiating sample, one must either sacrifice spectral resolution or collection efficiency. Tissue spectroscopic measurements, especially those made through an endoscope, would be greatly improved by using a fiber bundle to collect a larger portion of sample light. We achieve this with a scheme to recover the measured intensity distribution at the detector plane from the input fiber bundle.

In a conventional spectrometer or imaging spectrometer, light from an input aperture (such as a fiber or slit) is collimated, angularly dispersed by wavelength using a dispersive optical element such as a diffraction grating, and focused onto a detector. By focusing the angularly dispersed light, wavelength is mapped to position at the detector plane. However, the actual intensity distribution at the detector plane is a convolution of the input aperture with the power spectrum. For this reason the spectral resolution requires an input aperture which is as narrow as possible in the lateral dimension to allow an unambiguous mapping of wavelength to position at the detector plane.

A few groups have focused on using a collection of fibers as an input, arraying the fibers in a row at the input slit of an imaging spectrometer [1]. This approach, however, is still limited by the effective slit width and does not increase the throughput of an imaging spectrometer.

One scheme to allow for wider apertures, proposed by Gehm et al. and termed multimodal multiplex spectroscopy, involves imposing a certain intensity pattern or mask on the input aperture [2]. The mask is defined by a Hadamard matrix (a binary pattern of rows which are mutually orthogonal). Because the rows are orthogonal, its autocorrelation in the horizontal direction is a delta function. Thus, by performing a cross-correlation of the measured intensity pattern at the detector plane of the spectrometer with a copy of the Hadamard matrix aperture, the cross-correlation of the aperture with the analysis function reduces to a delta function, leaving only the power spectrum. Such a scheme has been designated “coded aperture spectroscopy”.

However, the Hadamard matrix is not the only family of aperture patterns which have this property. Any pattern whose rows are mutually orthogonal yields a delta function upon autocorrelation in the horizontal direction. Here we describe another method for generating a pseudo-orthogonal mask using only the output of a fiber bundle, which makes it ideal for adaptation to a fiber endoscope.

II. Background

Previous masking patterns have focused on binary intensity patterns, as these kinds of masks are simple to

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fabricate. However, there are many possible schemes involving continuously varying masks as well. A series of sine or cosine waves of different frequencies is also orthogonal. In cross section, the output of a bundle of fibers approximates a sine wave, with peaks at the center of each fiber and troughs in the borders. In order to generate a pseudo orthogonal series, one needs to alter the spatial frequency of fibers along one dimension. This can be accomplished in a purely optical fashion by applying distortion to the image of the fiber bundle, such as pincushion distortion. This kind of distortion introduces a nonlinear mapping along the radial coordinate of points on the input plane to points on the detector. This distortion of the image must be introduced before the dispersive element of the spectrometer to allow decoupling of input spatial position and wavelength.

A summary of these ideas is presented in Fig. 1. Fig. 1A and B shows an undistorted fiber bundle image and its autocorrelation function. It is immediately obvious that any spectrum convolved with this function will be unacceptably degraded. A sharp central peak is realized, but the function contains numerous confounding side lobes which introduce unacceptable ambiguity into the recovered power spectrum. Fig. 1C shows the image of the fiber bundle with simulated pincushion distortion. Its autocorrelation is now sharp with almost no side lobes (Fig. 1D).

It is easy to see that the recovery process relies upon very accurate knowledge and characterization of the input aperture function. This is accomplished by centering the image of the aperture on the detector while illuminating with a spectrally narrow line source. We prefer a gas atomic emission lamp as opposed to a coherent source to reduce speckle

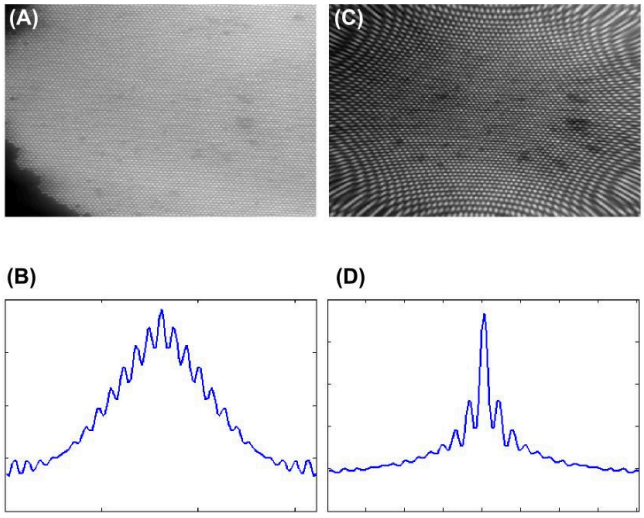

Figure. 1. Simulation showing narrowing of input fiber bundle autocorrelation function through pincushion distortion. (A) An image acquired of a portion of the face of a fiber bundle. (B) Autocorrelation of (a) in horizontal direction. (C) Simulated pincushion distortion applied to (a), varying the spatial frequencies of the fiber images. (D) Autocorrelation of (c) in the horizontal direction, with a narrower distribution due to the distortion.

artifacts, which introduce noise into the deconvolution analysis.

III. Method

The feasibility of spectroscopy from a fiber bundle was demonstrated with a calibration spectrum. We generate the input aperture pattern as follows: The output of a fiber bundle was magnified by a 10X objective (Newport). This image was then relayed by a small, high index plano-convex lens (1.5 mm diameter, 0.85 mm radius of curvature, LaSFN9, Opto-Sigma). This lens was chosen to introduce a large amount of pincushion distortion. Another 10X objective (Newport) then relayed the distorted image of the fiber bundle to the input plane of a custom built imaging spectrometer. The dispersive element was a 600 lines per millimeter ruled transmission grating (Thorlabs). A high resolution CCD camera was used as the detector (Photometrics Cascade 650, 653x492 pixels, 7.4 x 7.4 µm pixel size). The imaging spectrometer had a theoretical spot size of 10 µm at the detector.

An isolated spectral line from a calibration lamp was used to characterize the exact pattern of the distorted fiber image. We chose the atomic emission line at 587.1 nm from a krypton lamp (Oriel/Newport). The test spectrum was provided by a mercury-argon lamp, utilizing very two closely spaced lines (577.0 nm and 579.1 nm) (Ocean Optics).

The fiber bundle image contains an undesirable background intensity profile in addition to the high spatial frequency image of the individual fibers. This was removed by high passing the 2D Fourier transform of each collected image to remove low spatial frequencies and de-trend them.

IV. Results

Fig. 2A shows the detector plane image of a fiber bundle illuminated by only one wavelength from a spectral calibration lamp. Pincushion distortion has been deliberately introduced between the fiber output and the input plane of the imaging spectrometer, resulting in a nonlinear radial mapping of the image of the fiber bundle. This input pattern yields a result very close to the desired delta function upon autocorrelation in the lateral direction (Fig. 2B).

After characterizing the input pattern with a single wavelength calibration source (the 587.1 nm line from a krypton lamp), a test spectrum containing two spectral lines (577.0 and 579.1 nm from a mercury argon lamp) was recovered (Fig. 2C and D). This demonstrates recovery of two very closely spaced lines. Note that because the spectral lines were so close together, by visual inspection one cannot tell whether the detector image contains one or two copies of the input pattern because the images are nearly completely overlapped. (The partial image on the left side is from a third spectral line at 546.1 nm).

We also demonstrated the ability of this method to acquire Raman spectra. The sample was a cuvette of benzene, which has a well characterized spectrum. The excitation source was a blue diode laser (476 nm, 66 mW power, Laserglow). Raman scattered light was filtered with a longpass filter to

remove pump light and collected at 90° to the excitation beam with a 10X objective (0.25 NA, Newport). A camera integration time of 60 seconds was used to acquire a spectrum. The recovered spectrum is shown in Fig. 3A. Benzene's characteristic C–H stretch peak appears around 3050 cm^{-1}.

One key advantage of using a fiber bundle to collect spectral data is the ability to efficiently collect light from highly scattering samples. We demonstrated this by preparing a solution of benzene with titanium dioxide nanoparticles. The resulting solution transmitted ~4.5% of incident light after a 1 cm long cuvette ($\mu_s \approx 3.1$ cm^{-1}). Fig. 3B shows recovery of benzene signal from this sample.

CONCLUSION

We have demonstrated a scheme for recovering a spectrum from a slit-less imaging spectrometer with a fiber bundle input. Sub-nanometer spectral resolution was achieved, with clear differentiation of spectral features an order of magnitude smaller than the apparent image of the fiber bundle at the detector plane.

This approach has a number of advantages over other forms of coded aperture spectroscopy. A binary intensity mask such as that previously described by Gehm et al. throws away half the collected photons. No microscopic masking need be fabricated and aligned over the fiber bundle output ; the pseudo-orthogonal pattern is generated in a purely optical fashion. This allows us to work with all of the light collected from the sample. Finally, fiber bundles are ideally suited for adaptation to endoscopic applications.

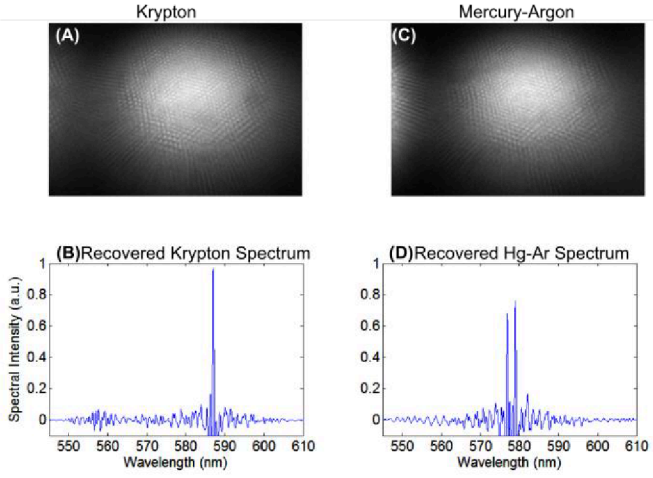

Figure. 2. Recovered test spectra. (A) Image at the detector plane of the imaging spectrometer of the distorted fiber bundle illuminated by a singlet (587.1 nm) from atomic krypton emissions and its recovered spectrum, (B). (C) Image at the detector when the fiber bundle was illuminated by a closely spaced doublet (577.0 and 579.1 nm) from a mercury-argon lamp. (D) Recovered spectrum demonstrating clean separation of the doublet.

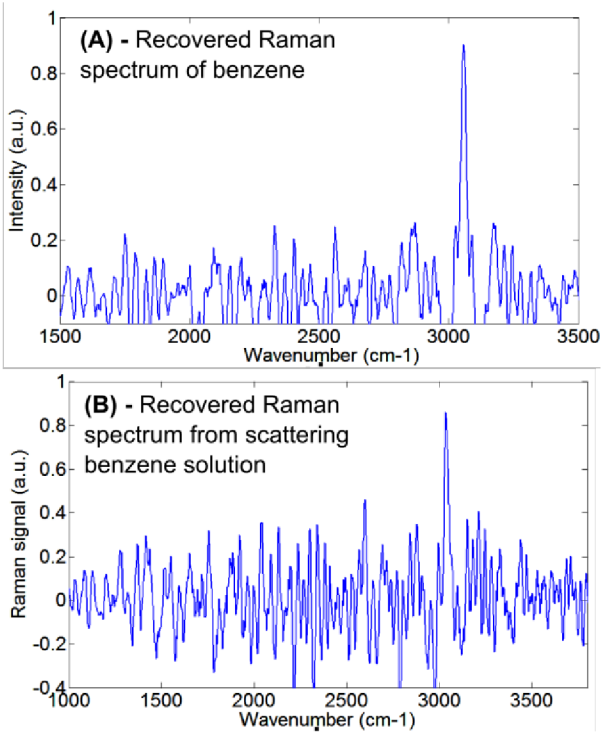

Figure 3. (A) Recovered Raman spectrum of benzene, showing characteristic C–H stretching peak around 3050 cm^{-1}. (B) Recovered Raman spectrum of benzene from a highly scattering solution.

REFERENCES

[1] J. Ma, and D. Ben-Amotz, "Rapid Micro-Raman Imaging Using Fiber-Bundle Image Compression," Appl. Spectrosc. **51**, 1845-1848 (1997).

[2] M. E. Gehm, S. T. McCain, N. P. Pitsianis, D. J. Brady, P. Potuluri, and M. E. Sullivan, "Static two-dimensional aperture coding for multimodal, multiplex spectroscopy," Appl. Opt. **45**, 2965-2974 (2006).