



Introduction

Raman spectroscopy is a type of vibrational spectroscopy in which a laser beam is used to excite a particle and cause molecular vibration. From this vibration, a "molecular fingerprint" can be deduced, and the molecule can be identified.

When using Raman spectroscopy, particles must first be detected before they are analyzed. Proper detection relies on the concept of contrast, in which the particle being analyzed and the substrate are clearly distinguishable. Contrast is achieved through using the correct illumination source; if illumination is used improperly, it can result in damaging or incorrectly identifying the sample (Tripathi et al., 2011).

Using different substrates, or backgrounds, can make particle detection more challenging. When substrates are various colors, finding the optimal illumination wavelength may become difficult (Emmons et al., 2009). However, using different substrates makes particle detection more applicable to fields such as forensics. The purpose of this project was to detect explosive samples on substrates of different colors using Raman spectroscopy.

Materials and Methods

%¹⁰⁰ In this experiment, three red, blue and green cotton strips were used. First, an initial experiment was run to determine the reflectivity of each substrate to hypothesize which LEDs would detect the most particles on each substrate. Using the Agilent Cary WinUV spectrometer, the percent reflectivity was calculated for each substrate, and a total of five trials were run per substrate. In 200 000 Wavelength (nm) each trial, the spectrometer was placed on a section of the **- - -**625 nm LED ---565 nm LED -Green Cotton substrate, with care taken to make sure the surface was smooth and Graph 1 (above): The percent reflectance values for the cotton substrates and the intensity values stable. In between trials, the spectrometer was placed on a for the LEDs. All the LEDs have no intensity until they peak at their relative wavelengths, whereas the cotton substrates have steadily decreasing reflectance until they have a more subtle peak different section of the substrate to ensure that results reflected the around their respective color on the visible light scale. substrate in its entirety. The explosive sample, which consisted of Comparison of experimental spectra versus library a mixture of the explosives RDX, HMX, and potassium chlorate spectra (PC), was then deposited onto the substrates. Raman spectroscopy **S** 2500 **Un** 2000 was run using the Pendar Portable microscopy chemical detection > 1500 system (PMCDS). The illumination wavelength was changed rbi using the CHLORIS LED instrument. Two trials of each 1575 illumination wavelength were performed on each substrate, as well Wavenumber (cm⁻¹ as all three LEDs being shined at once. Figures 1 through 3 display - - RDX Library Spectra - - PC Library Spectra - - Average Spectra 3 LED Graph 2 (above): A comparison between the experimental spectra of RDX, HMX, PC, and the how one of the substrates, Blue Cotton 1 (BC 1), looks underneath spectra of the correctly identified particles of the BC1 substrate under the illumination of all each illumination wavelength. three LEDs.

Detecting explosive samples on colored substrates with Raman spectroscopy Radha Kausik

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Materials and Methods (continued)



Figure 1 (above): BC1 under 475 nm illumination.



Figure 2 (above): BC1 under 565 nm illumination.



Results

The results of the initial reflectance experiment determined that the best illumination values to use are 475 nm (blue), 565 nm (green), and 625 nm (red). The reflectivity and intensity values are displayed in Graph 1. Graph 2 showcases the library Raman spectra of the explosives used in this experiment, and the average spectra of the successfully identified particles of the substrate BC1 under each illumination wavelength. Graph 3 displays the success rates of the Raman spectroscopy for each substrate and illumination value. A Raman spectroscopy reading was considered a success if it correctly identified a particle as RDX, HMX, or PC.







Results (continued)

Success rates of Raman Spectroscopy with multiple illumination sources



Graph 3 (above): The success rates of the Raman spectroscopy reading. The blue cotton substrate (BC) proved to have the lowest success rates (n = 18, M = 19.33, SD = 9.43), the red cotton (RC) substrate had a marginally higher success rate (*n* = 18, M = 51.11, SD = 12.37), and the green cotton substrate had the highest and most consistent success rate (n = 18, M = 60.00, SD = 7.94).

Conclusions

The purpose of this project was to detect explosive samples on substrates of different colors using Raman spectroscopy. The results from the Raman spectroscopy revealed that LED colors that contrasted with the substrate color yielded the most particles detected and identified accurately. This was consistent with Graph , as the reflectivity values indicate that contrasting LED colors will correctly identify the most particles.

The results found could prove useful in creating more Additionally, these results make particle detection in fields such

automated Raman spectroscopy devices. With the data on contrast gained from this project, it is possible to program a Raman spectroscopy device to automatically generate this contrast and therefore make detecting particles a much easier process. as forensics more straightforward. The data on substrates can be applied to more common substrates such as denim and nylon. From there, proper illumination contrast techniques can be used to achieve the most accurate particle detection and identification.

References

Emmons, E. D., Tripathi, A., Guicheteau, J. A., Christensen, S. D., & Fountain, A.W., III (2009). Raman chemical imaging of explosive-contaminated fingerprints. Applied Spectroscopy, 63(11), 1197–1203. https://doi.org/10.1366/3702097898012 Tripathi, A., Emmons, E. D., Wilcox, P. G., Guicheteau, J. A., Emge, D. K., Christesen, S. D., & Fountain, A.W., III (2009). Semi-automated detection of trace explosives in fingerprints on strongly interfering surfaces with Raman chemical imaging. *Applied* Spectroscopy, 65(6), 611–619. https://doi.org/10.1366/10-06214



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