

Performance Analysis of Raman LiDAR over Raman Spectroscopy for Detecting Remote Trace Explosives

Aishwarya Singh^{*}, Anupama Bhattacharya^{**}, Sangeetha N^{***}, S. Rajalakshmi^{****}

^{}School of Electronics Engineering, VIT University*

*^{**} School of Electronics Engineering, VIT University*

*^{***} School of Electronics Engineering, VIT University*

*^{****} School of Electronics Engineering, VIT University*

ABSTRACT

The aim of this paper is to analyze the performance of Raman Light Detection and Ranging (LiDAR) technique and Raman Spectroscopy technique to detect trace explosives such as Research Department Explosive (RDX) and Trinitrotoluene (TNT). In various situations, when explosives are prepared, transported or handled, a quantifiable amount of explosive material ends up on surfaces. The main focus lies on the comparison between the two techniques for detecting these traces. This paper is based on the design of Raman LiDAR so that it can be used for real time application, keeping in mind the commercially available fibers. The merits and demerits of both the techniques have been studied. We are investigating which method is best suited for detecting remote trace explosives.

INDEX TERMS- Attenuation, Doppler shift, Explosive, Multimode fiber, Raman LiDAR, Raman shift, Raman spectroscopy, RDX, TNT.

1. INTRODUCTION

In the recent years various detection techniques have been developed to detect traces of explosives. There are mainly two types of detection techniques that is remote detection and standoff detection. In remote detection, the personnel performing explosives screening maintains a safe distance from the item being screened, but the screening equipment does not. However, in standoff detection, the personnel and equipment are at a safe distance from the explosive. We are focusing on standoff detection using Raman Effect. This effect involves analyzing the backscattered light and calculating the Raman shift which gives a fingerprint of the explosive. The design of Raman LiDAR is proposed for real time application. Raman LiDAR is a modified

version of Raman spectroscopy. Both these techniques work on the principle of Raman Effect. A detailed comparison between the two techniques is studied. A major advantage of LiDAR over spectroscopy is its high precision, safety, accuracy and higher range of detection. But the basic advantages of Raman spectroscopy are its non destructive character and high sensitivity.

2. SOFTWARE USED

The software used here is Optisystem 13. OptiSystem is a comprehensive software design suite that enables users to plan, test, and simulate optical links in the transmission layer of modern optical networks.

3. WORKING PRINCIPLE

A. Raman Spectroscopy

There are two types of scattering, elastic (no change in the frequency of the emitted photon) and inelastic (change in the frequency of the photon after scattering). Raman spectroscopy is a spectroscopic technique based on inelastic scattering of monochromatic light, usually from a laser source. Photons of the laser light are absorbed by the sample and then reemitted. Frequency of the re-emitted photons is shifted up or down in comparison with original monochromatic frequency, which is called the Raman Effect. This shift provides information about the chemical composition of the explosive. The Raman interaction leads to three possible outcomes. First, the material absorbs energy and the emitted photon has a lower energy than the absorbed photon. This outcome is labeled Stokes Raman scattering, (Red shift). Second, the material loses energy and the emitted photon has a higher energy than the absorbed photon. This outcome is labeled anti-Stokes Raman scattering, (Blue Shift). Third, the material absorbs a photon, the excited molecule returns back to same vibration state and emits light with same frequency. This outcome is labeled Rayleigh scattering. [15]



Figure 1: Three possible outcomes of Raman interaction.

A. Raman LiDAR

The principle behind Raman LiDAR is similar to Raman Effect. When a light is focused on a surface, it measures the time to return to its source. The LiDAR instrument fires rapid pulses of laser light up to 150,000 pulses per second. [9] A sensor on the instrument measures the amount of time it takes for each pulse to bounce back. Light moves at a constant and known speed so the LiDAR instrument can calculate the distance between itself and the target with high accuracy. By repeating this process at a high speed, the instrument builds up a complex map of the sample. There are two types of LiDAR detection method, coherent detection and incoherent detection. Coherent detection method is best used for Doppler shift measurements. It operates at lower but it is expensive due to its complex transceiver. The most prominent advantage of that the low powered lasers provide eye safety and hence can be used with little precautions. [9] Incoherent detection is used for atmospheric research such as height, layering and density of clouds, cloud particles properties, temperature, pressure, wind, humidity and trace gas concentration.

B. Block diagram

The basic block diagram for both the techniques is similar. The focusing and collecting optics of LIDAR cause less attenuation as compared to spectroscopy. Also a major difference between the two techniques is the detector used. The four major components of Raman LiDAR are (1) Lasers (2) Scanners and Optics (3) Photo detector (4) Navigation and positioning systems. [9]

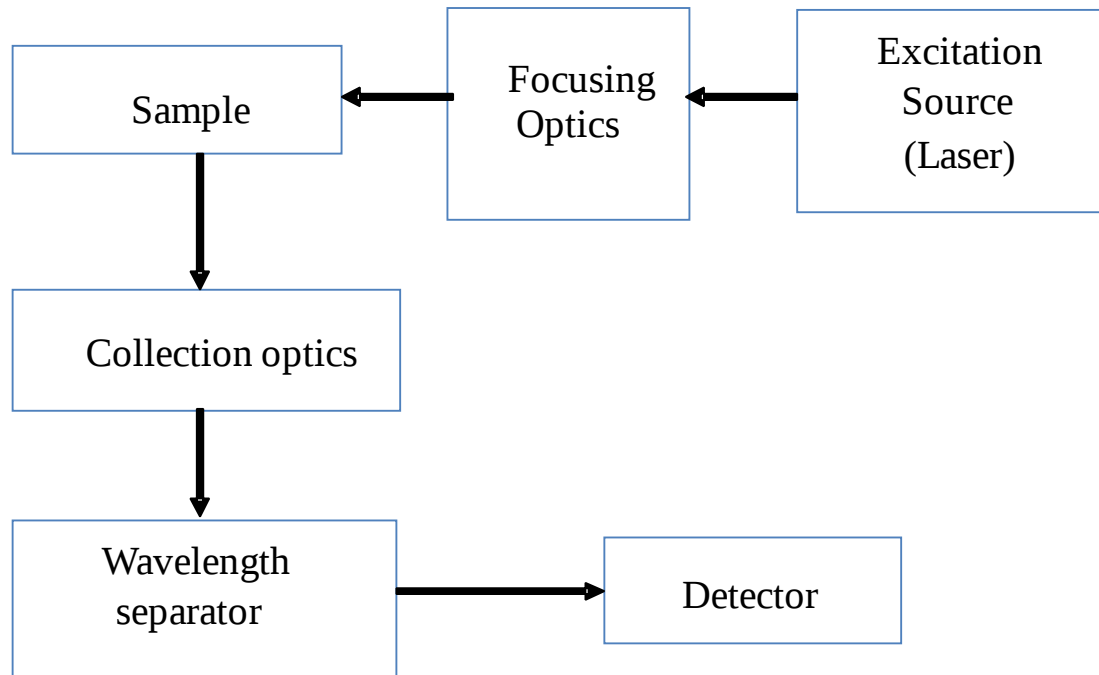


Figure 2: Block diagram for detection technique.

In both the cases, a laser of suitable wavelength acts as an excitation source which is focused on the sample, placed at a distance of few meters. In LiDAR, a telescope is used to maximize the output from the laser whereas; a combination of mirror and lens is used in spectroscopy. Telescope provides lesser attenuation and higher precision rate. The shifted wavelength is then converged through the collection optics onto the detector. A multimode fiber is used as the collection optics and photo detector or photo multiplier acts as a detector in LiDAR while lens as an optics and spectrum analyzer as a detector is used in Spectroscopy.

4. EXPLOSIVE

Explosives may be broken down into two general classes: nitro/nitrate-based and non-nitro/nitrate-based. Non-nitro/nitrate-based explosives are derived from materials such as peroxides, e.g., tri-acetone tri-peroxide (TATP), per chlorates, and azides. While these explosives clearly pose a threat, our studies focused upon the more common nitro-based explosives. The nitro based explosives include Research Department Explosive (RDX), Trinitrotoluene (TNT) and PETN. Nitro-based explosives have at least one NO_2 group. When they detonate, one of the end products is N_2 gas, which is very stable due to its N-N triple bond. The formation of this low-energy product is accompanied by the release of a sizable amount of energy. [3]

A. Trinitrotoluene (TNT)

TNT, or trinitrotoluene, is the most important military explosive. It is very stable and can be stored for long periods. It is extremely moisture resistant and is not likely to be detonated by physical shock. [17]

B. Research Department Explosive (RDX)

RDX, an acronym for Research Department Explosive, is chemically named cyclo-trimethylene-trinitramine. It is a handy and versatile material for bringing about all kinds of destruction. It is frequently used in blasting caps. [17]

5. RAMAN LIDAR DESIGN

The excitation source used here is Neodymium-Yttrium (Nd-Yag) laser (532nm). Nd-Yag laser (532nm) falls within the visible spectral region where optical components are easily available and affordable making it uncomplicated to design the instrumentation. It can be used under harsh weather conditions. When a single Nd-Yag laser is used a sharp Raman peak is not obtained. However when two laser beams are used a sharper peak is obtained. Due to software constraint, a telescope couldn't be designed. Hence, a fiber Bragg grating and thin lens are used. . A fiber Bragg grating is a distributed Bragg reflector that reflects particular wavelengths of light and transmits all others. Therefore, it can be used as an inline optical filter to block certain wavelengths, or as a wavelength-specific reflector. The filtered wavelength is then converged through a thin optical lens. The converged output passes through a multimode fiber. A multimode fiber is preferred because the application here is short

distance based. Multimode fibers have large core diameter as compared to single mode fibers. Hence, the signal loss is comparatively low. Graded index multimode fiber is chosen over step index multimode fiber in order to reduce modal dispersion. The refractive index of the core of the graded index fiber is maximized at the center of the core and then it decreases towards core-cladding interface. Exploring a variety of commercially available multimode fibers from Newport Corporation and Thorlabs Inc, a multimode graded index fiber GIF 625 which matches the design specifications was chosen. The design requirements and calculation are discussed in the following sub section. [16]

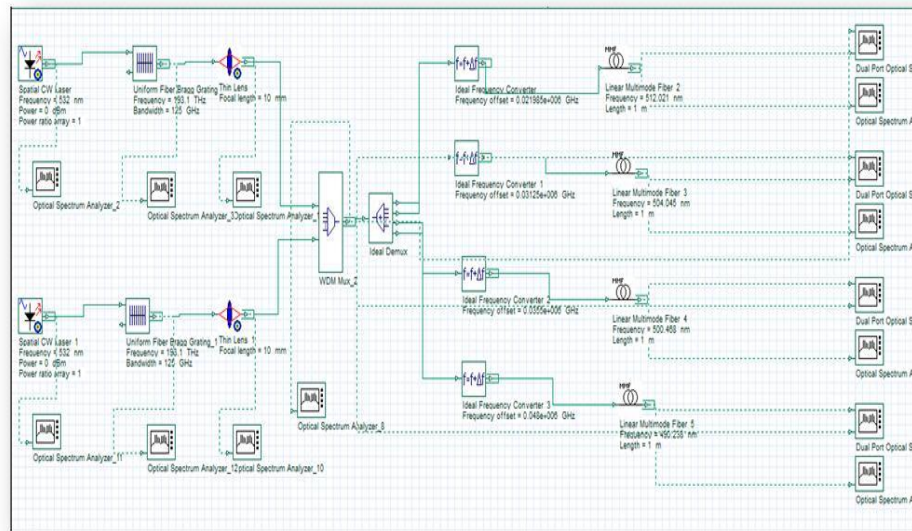


Figure 3: Raman LiDAR design

A. Acceptance angle and Numerical Aperture

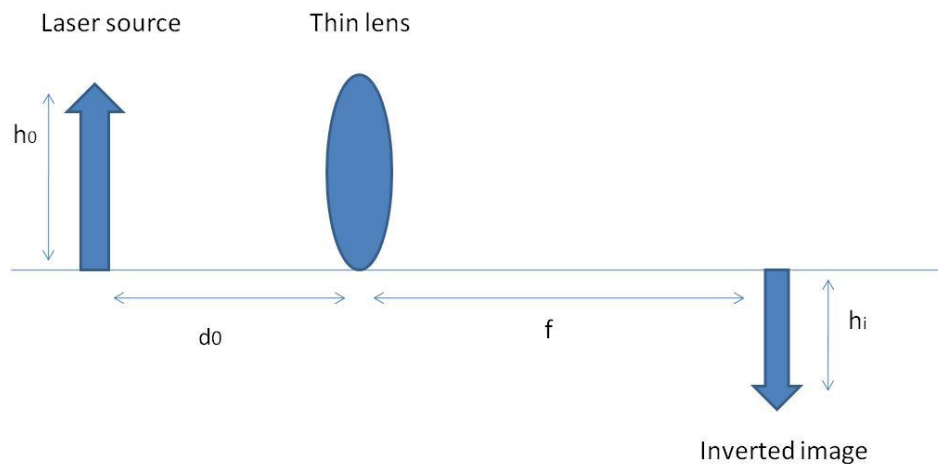


Figure 4: Height of the image calculation..

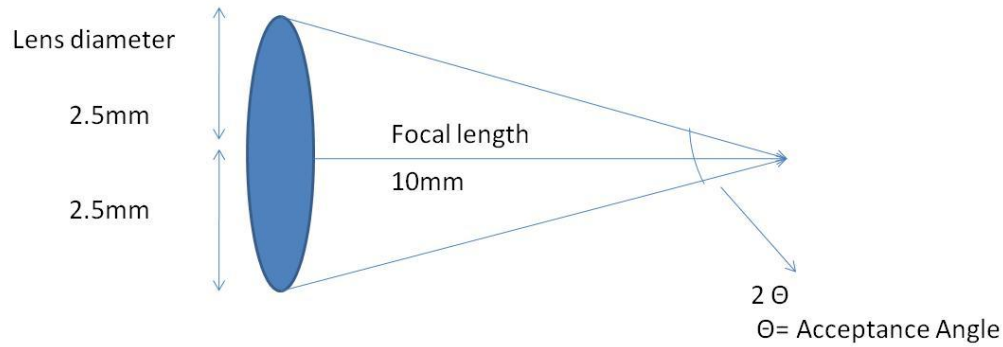


Figure 5: Acceptance angle calculation

By Pythagoras theorem,

$$10^2 + (2.5)^2 = c^2$$

$$c = 10.307764$$

$$\sin \theta = \frac{2.5}{10.307764}$$

$$= 0.2425$$

$$\theta = 14.3034 \text{ degrees}$$

Where, θ is the acceptance angle.

$$\text{Numerical Aperture (NA)} = n \sin \theta$$

$$= 1 * \sin(14.3034)$$

$$= 0.2429$$

Here, air is the medium. Therefore, refractive index (n) = 1

$$\frac{h_i}{h_o} = -\frac{d_i}{d_o}$$

$$\frac{h_i}{5 * 10^{-3}} = -\frac{10 * 10^{-3}}{1}$$

$$h_i = -50 * 10^{-6}$$

$$h_i = -50 \mu\text{m}$$

The height of the image is found to be 50 μm and the negative sign indicates that the image is inverted. The fiber length is 1m.

It can be concluded from the above design analysis that the required numerical aperture is 0.24. However, Thorlabs provides graded index multimode fibers with numerical aperture 0.22 and 0.27. Numerical aperture of 0.27 was chosen for our design. The core diameter of the multimode fiber corresponds to the height of the image through the lens. The core diameter calculated is 50 μm which is close to the commercially available 62.5 μm multimode fiber available at Thorlabs. [16]

B. Fresnel's coefficients

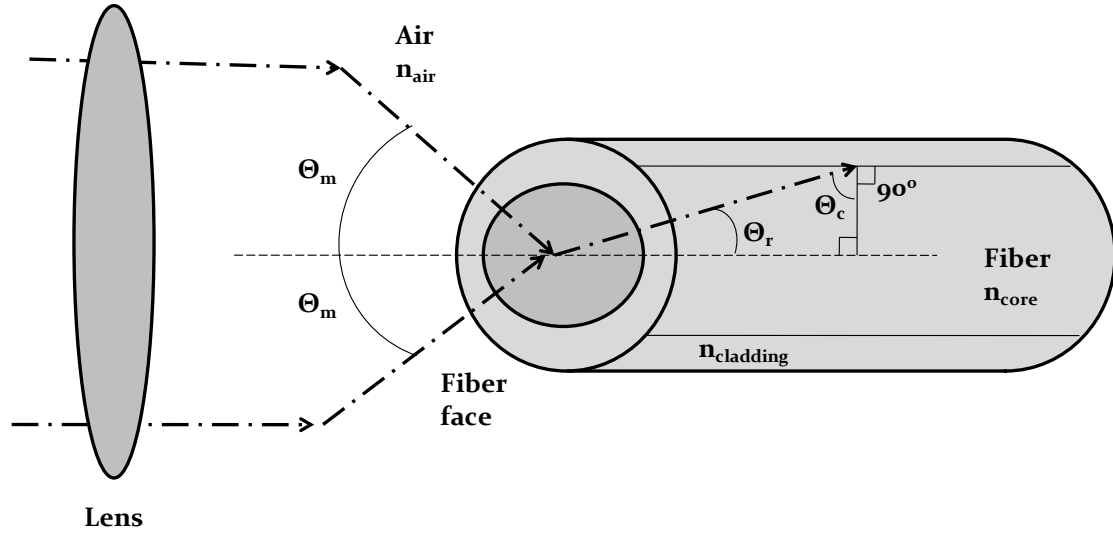


Figure 6: Fresnel transmission and reflection coefficients calculation.[6]

$$N_{core} = 1.48585$$

$$N_{cladding} = 1.45641$$

At the core cladding interface,

$$\theta_c = \sin^{-1}\left(\frac{N_{cladding}}{N_{core}}\right)$$

$$\theta_c = \sin^{-1}\left(\frac{1.45641}{1.48585}\right)$$

$$\theta_c = 78.5755 \text{ degrees}$$

According to right angle geometry,

$$\theta_r = 90 - 78.5755$$

$$\theta_r = 11.1904 \text{ degrees}$$

By Snell's Law, at fiber interface,

$$N_{air} * \sin(\theta_m) = N_{core} * \sin(\theta_r)$$

$$1 * \sin(\theta_m) = 1.48585 * \sin(11.4245)$$

$$\sin(\theta_m) = 0.28837$$

$$\theta_m = 16.76 \text{ degrees}$$

Parallel Transmission (t_p) and reflection coefficient (r_p) of the fiber is [11, 12]

$$t_p = 2 * n_1 * \frac{\cos\theta_3}{((n_1 * \cos\theta_4) + (n_3 * \cos\theta_3))}$$

$$t_p = 0.79669$$

$$r_p = \frac{(n_3 * \cos\theta_3) - (n_1 * \cos\theta_4)}{(n_1 * \cos\theta_4) + (n_3 * \cos\theta_3)}$$

$$r_p = 0.18377$$

Power Transmission %= 96.6226%

Power Reflection %= 3.37735%

6. FIGURES AND TABLES

Table 1: Examples of Red shift and Blue shift.[5]

Vibrational Mode Assignment	Explosive (Type)	Wavenumber (cm ⁻¹)	Shifted Wavelength (nm)
NO ₂ deformation and ring stretch	Nitramine(RDX), TNT	650-850	510-513
N-N Stretch	Nitramine(RDX)	1200-1230	499-504
NO ₂ symmetric stretch	Nitramine(RDX)	1260-1320	499-501
NO ₂ asymmetric stretch	Nitramine(RDX), TNT	1450-1600	490-491

The table shows the numerical values of Red shift and Blue shift of different chemical constituents when they are excited by a laser of 532nm.

Table 2: Wave number ranges and vibrational mode assignment of spectra of explosives.

Raman Wavelength & Wavenumber Solver Chart										
Excitation Laser				532	nm			18,797	cm ⁻¹	
Shift (cm ⁻¹)			Group	Intensity	Red Shift(nm)			Blue Shift(nm)		
100	-	210	Lattice Vibration	Strong	534.8	-	538.0	529.2	-	526.1
150	-	430	Xmetal-O	Strong	536.3	-	544.5	527.8	-	520.1
250	-	400	C-C Aliphatic Chain	Strong	539.2	-	543.6	525.0	-	520.9
295	-	340	Se-Se	Strong	540.5	-	541.8	523.8	-	522.5
425	-	550	S-S	Strong	544.3	-	548.0	520.2	-	516.9
450	-	550	Si-O-Si	Strong	545.0	-	548.0	519.6	-	516.9
490	-	660	C-I	Strong	546.2	-	551.4	518.5	-	514.0
505	-	700	C-Br	Strong	546.7	-	552.6	518.1	-	512.9
550	-	790	C-Cl	Strong	548.0	-	555.3	516.9	-	510.5

The table above has a list of different components present in RDX and TNT. It also shows their shifted wavelength and the amount of shift in their wave number.

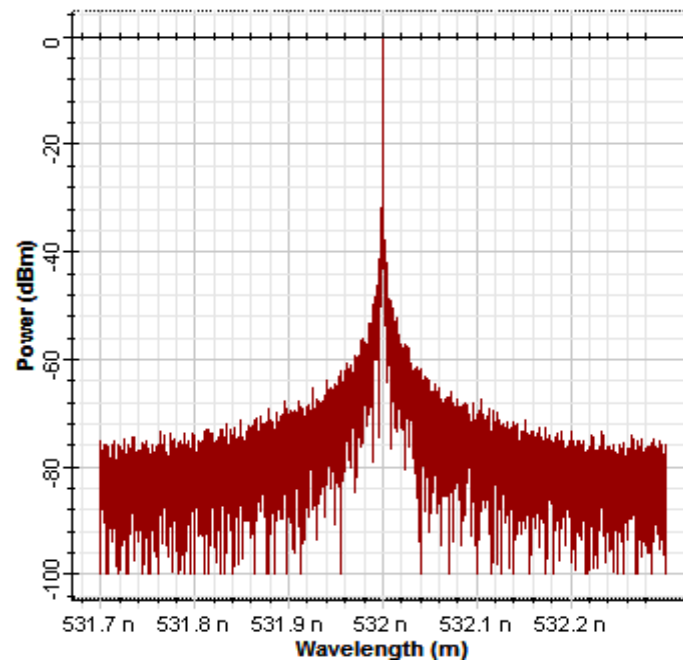


Figure 7: Input from the Nd-Yag laser source (532nm).

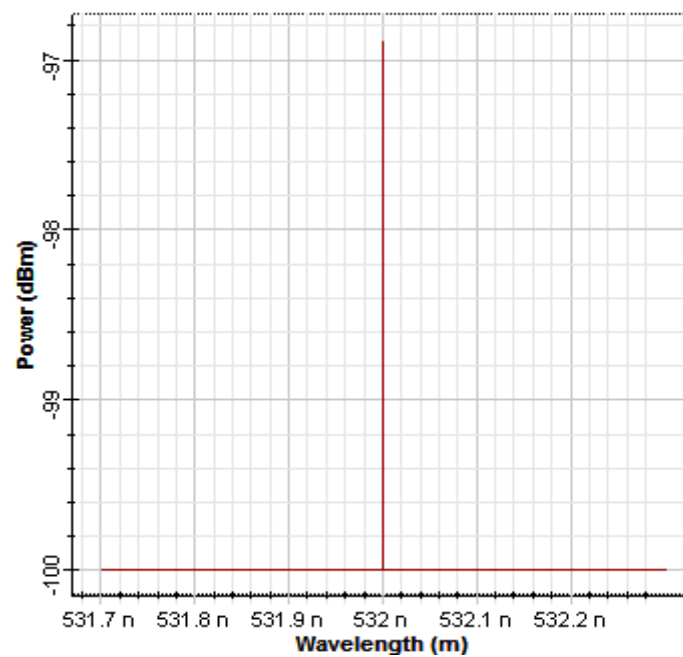


Figure 8: Sharp peak obtained after passing the laser beam through the focusing optics.

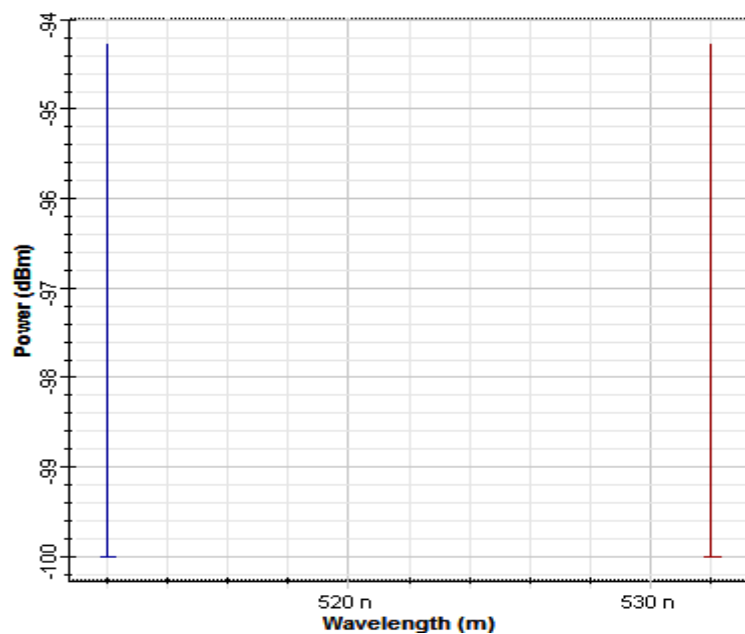


Figure9: NO₂ Deformation and Ring Stretch (RDX, TNT)

The presence of NO₂ Deformation and Ring Stretch in RDX, TNT gives a shifted wavelength of ~512nm which corresponds to shift in wave which is 725cm^{-1} . Hence a sharp peak is obtained at 512nm.

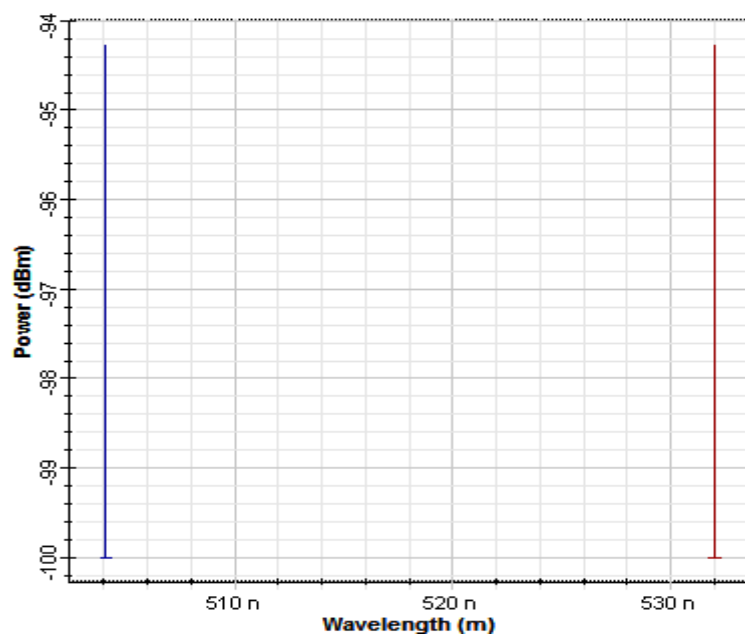


Figure 10: N-N Stretch (RDX)

Similarly like the above two shifts a blue shift of approximately 1200cm^{-1} helps to detect N-N Stretch in RDX. The shift in wavelength corresponds to 504nm.

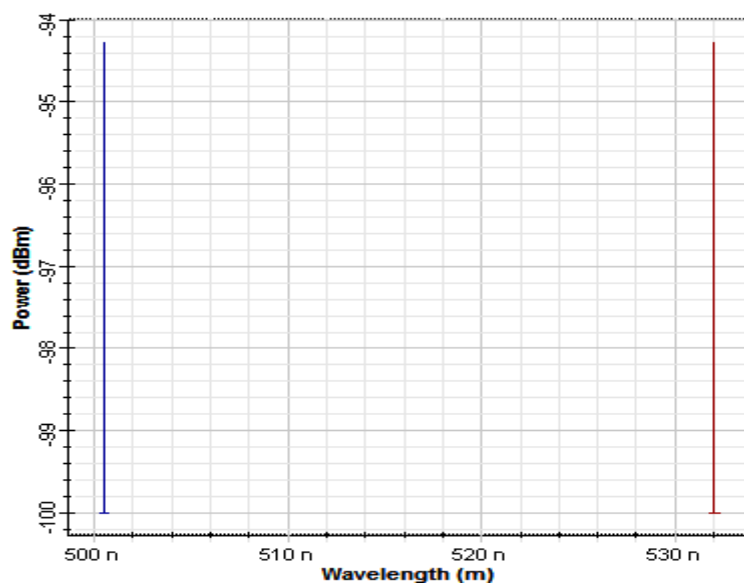


Figure 11: NO₂ Symmetric Stretch (RDX)

Here the shifted wavelength is nearly 500nm which corresponds to a shifted wave number of 1300cm^{-1} . Hence, it can be concluded that NO₂ Symmetric Stretch is present in RDX.

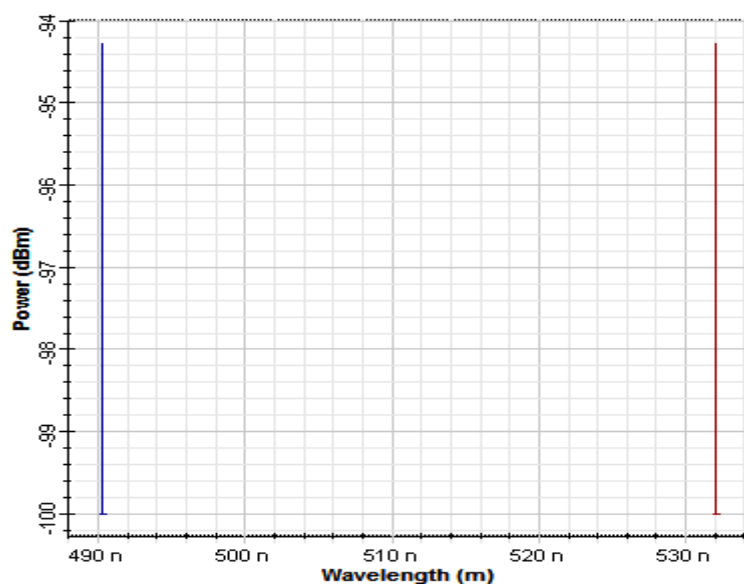


Figure 12: NO₂ Asymmetric Stretch (RDX, TNT)

The initial wavelength of 532nm has been shifted to ~490nm. The shifted wavelength gives the corresponding wave number which is used to determine the component in the explosive. Here NO₂ Asymmetric Stretch in RDX, TNT.

7. CONCLUSION

We have proposed a compact design of Raman LiDAR to detect remote trace explosives over the conventional Raman spectroscopy technique. The major difference between the two techniques is that in Raman spectroscopy the scattered spectra of light is analysed whereas in Raman LiDAR the photon count after scattering is taken into account. The telescope used in Raman LiDAR gives higher precision, lower attenuation and high accuracy. In contrast, Raman spectroscopy uses a numerous of combination of lens and mirror which contribute to linear and non linear scattering losses. Lasers with a wavelength of 1550nm are a common alternative for 532nm as they are not focused by the eye and are 'eye-safe' at much higher power levels. These high wavelengths are used for longer range and lower accuracy purposes. Another advantage of 1550nm wavelengths is that they do not show under night-vision goggles and are therefore well suited to military applications. But CCD detectors are not very good into the infrared past 1100nm and are very slow. Raman LiDAR has a wide range of operation as compared to Spectroscopy. There is a trade off between the accuracy and cost of the Raman LiDAR. . One major area of improvement is using an excitation source which has wavelength in the UV range. Since a Raman signal is inversely proportional to the fourth power of the incident laser radiation wavelength, the latter must be in the UV range to yield the strongest Raman intensity. To add to it, 532 nm is not the optimal Raman probing wavelength because fluorescence often occurs in this spectral region. The Raman signal intensity scales with $1/\lambda^4$, leading to the conclusion that UV wavelengths would be the better choice.[4] However, 532 nm falls within the visible spectral region where optical components are easily available and affordable, making it flexible enough to design the experimental setup or instrumentation.

Table 3: Comparison of laser methods of standoff detection of explosive traces in the form of particles on the surface of objects. [1]

Detection Method	Detection distance(m)	Selectivity	Eye Safety
LIBS (Laser Induced Breakdown Spectroscopy)	45-100	Intermediate	No
CARS (Coherent Anti-Stoke's Raman Spectroscopy)	12	High	No
Raman Spectroscopy	30	High	No
Raman LiDAR	500-50,000	High	Yes

8. FUTURE WORK

We suggest in making the system compact for it to efficiently work in the outdoor environment. The components of Raman LiDAR are sensitive and easily prone to damage if exposed to harsh environment. Hence, extreme protection must be provided to the fiber to make it sturdy. As it is one of the most important components of the Raman LiDAR design. Better means can be developed to make the excitation source eye safe.

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APPENDIX A

- 1. h_o - spot size (height) of the laser (5mm)
- 2. d_o - distance of the laser from thin lens (1m)
- 3. f - focal length (10mm)
- 4. h_i - height of the image (50 μ m)
- 5. θ - acceptance angle.
- 6. N_{core} -refractive index of core(Germanium doped)
- 7. $N_{cladding}$ -refractive index of cladding
- 8. θ_c - critical angle
- 9. θ_m - incidence angle of fiber
- 10. θ_r - refracted angle from the fiber