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Fast and safe detection of sensitive explosives via pulsed raman spectroscopy

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Abstract Raman spectroscopy is one of the most established methods for the rapid and reliable detection of explosives and other hazardous chemicals. It enables first responders to identify suspicious substances quickly and remotely, avoiding direct contact with potentially dangerous or explosive substances. Present systems available on the market nowadays are small and light enough for mobile use in many applications. However, the measurement of dark coloured substances like black powder or other sensitive explosives harbours the risk of ignition. This is particularly the case if the measurement spot is not changed during the procedure. High absorption of the laser energy usually leads to a strong heat development in the analysed material, leading to decomposition or even ignition of the substance. To overcome this challenge, this work focuses on experiments with a pulsed nanosecond laser with optimized repetition rate and beam fluence. Different sensitive explosive materials such as triacetone triperoxide (TATP), black powder and mixtures of both are irradiated with pulsed laser light to perform Raman analyses. Results show the capability of the presented method to obtain high-quality spectra in short measurement times without any observed ignition of the sensitive explosive material. In addition, the influence of ambient light on the detection performance is evaluated and can be minimized. Further efforts are being made to miniaturize the entire laboratory set-up in order to take first steps towards the development of a portable device.

1 Introduction

Raman spectroscopy as one of the most suitable tools for the fast and reliable detection of explosives and other hazardous chemicals in CBRNE-related events enables first responders to quickly identify unknown suspicious substances—both liquid and solid—over a wide range by recognizing their “chemical fingerprint”. The measurement can be taken contactless with no need for sample preparation procedures in case of open accessible samples, making it possible to avoid direct contact with potentially hazardous or explosive substances [1, 2]. In case of covered target substances, different adaptions of the Raman method are described in the literature. Spatially offset Raman spectroscopy (SORS), for example, can be used as a non-invasive technique to collect Raman spectra through diffusely scattering opaque materials by measuring at a localized distance from the irradiation area [3, 4]. Another approach is a combined laser drilling and spectroscopic method that we reported to gain Raman signals of concealed explosives through small bore holes in the micron range [5] In recent years, stand-off capabilities of Raman methods have been further improved and demonstrated, for example, in combination with surface enhanced Raman spectroscopy (SERS) in cases where only traces of target substances can be found [6].

Nowadays, systems are available compact and light enough for portable operations in many application fields [7]. However, the usage of these commercially devices often comes along with a strong recommendation to not point the laser to dark coloured substances or any other sensitive primary explosive material, especially when the laser spot position is not altered during the measurement. For continuous-wave lasers with significant high average optical power, the risk of ignition exists during the measurement [8]. Strong absorption of the laser beam typically leads to high accumulation of heat, which is discussed as a main influencing mechanism for ignition and combustion of the analysed material [9].

To overcome this challenge and to be able to analyse samples at one specific measurement spot, this research work focuses on experiments with a nanosecond pulsed laser with optimized repetition rate and beam fluence. Different explosive materials like triacetone triperoxide (TATP), black powder and mixtures of both substances are irradiated by the pulsed laser in order to perform Raman spectroscopic analyses. The aim of the presented work is to gain high-quality spectral data in preferably short measurement times without the risk of igniting the sensitive explosive material. In addition, the influence of ambient light on the detection performance is evaluated and countermeasures are undertaken to minimize the negative impact on the results. Reference studies are carried out using a continuous-wave (cw) laser with the same emission wavelength as the pulsed source in order to study ignition

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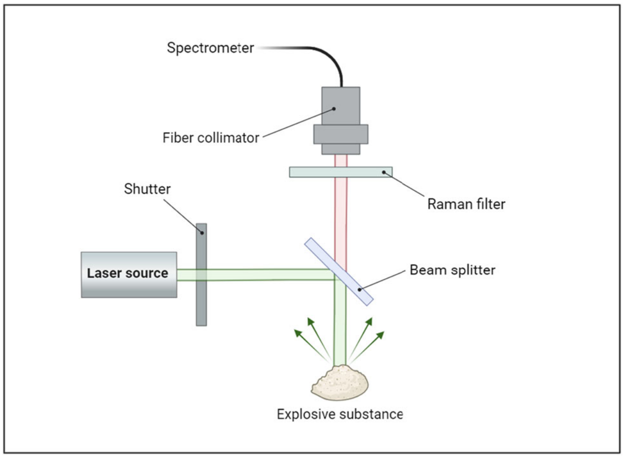


Fig. 1 Schematic sketch of the experimental setup: A pulsed Nd:YAG laser beam is guided to the explosive substance using a beam splitter. An integrated shutter is used to control the irradiation time. Backscattered light from the sample is lead to a spectrometer through a fiber collimator. A raman filter is used on this path to block the emission wavelength of the laser

thresholds and to show the principal ignitability of the different samples. Further efforts are made to miniaturize the whole laboratory set-up in order to take first steps towards the operation mode in portable applications for a potential commercial utilization.

2 Experimental set-up

A schematic overview of the set-up is shown in Fig. 1. A nanosecond pulsed laser with a central wavelength of 532 nm (*Crylas GmbH*) is used to irradiate different explosive samples without altering the measurement spot during the procedure. Pulse generation is done by passively Q-switching, leading to achievable pulse durations of less than 10 ns. The laser can be operated in different repetition rates from single shot up to 1 kHz. Single pulse energy of the laser is chosen to be constant at approximately 60 µJ with a laser spot diameter of 400 µm. The laser beam is guided to the sample by means of a beam splitter with transmissive characteristics for spectral signals beyond the excitation wavelength. All collected Raman signal is filtered by a long-pass filter (*Semrock*) and led to a spectrometer (*USB2000, Ocean Insight*) via a glass fibre with a core diameter of 600 µm (*Ocean Insight*). A shutter integrated in the laser source is utilized to control the irradiation time on the samples.

All Raman measurements are taken on different energetic substances prepared in special sample containers (produced by *ExploTech GmbH*), which enable reproducible preparation and simple decontamination of the used containers. The specimen consists of an inner cylinder with a diameter of 3 mm and a length of 5 mm containing the target substance. In this work, triacetone triperoxide (TATP), black powder and mixtures of both substances are used as explosive samples in different weight percentages. For TATP, the sample amount is about 15 mg and for black powder it lies in the 40–50 mg range, depending on the grain size of the powder and the grade of compaction.

In a second set-up—after the Raman analysis has been completed—all samples are irradiated with a continuous-wave (cw) laser (*Verdi V2, Coherent*) with a wavelength of 532 nm and a spot diameter of 2.2 mm, whereby the average power is increased stepwise to determine the ignition thresholds. In this set-up, all explosive substances are irradiated directly and without guiding or focusing of the laser beam. Since these experiments focus on the ignitability of the examined substances, no Raman spectra are captured during the irradiation with the cw laser.

3 Results and discussion

First experiments are carried out to analyse Raman response of the explosive substance triacetone triperoxide (TATP), which reacts very sensitive to electrical discharge, heat, friction and mechanical stress [10]. Results show the successful measurement of strong Raman signals without any observed ignition at different laser parameters with the pulsed system. During the measurements, the optical set-up is blocked from ambient light in order to get clean spectral data without any influences of other light sources than the laser. Exemplarily Raman spectra of TATP are shown in Fig. 2 for different pulse repetition rates (integration time 200 ms; 10 × averaging). The registered intensity is plotted against the calculated Raman shift in wavenumbers. Even at the lowest checked repetition rate (5 Hz), an analysable spectrum of TATP can be obtained. As the integration time of the spectrometer is set to 200 ms, this measurement represents the spectral signal of one laser pulse interacting with the sample. This illustrates the possibility of recording single shot Raman spectra with TATP as a target substance. Compared with a classical Raman spectroscopic approach using a cw laser, this can be seen as a remarkable result, since the interaction time of the laser light with the explosive material is minimized in this measurement. Also, a linear dependency between the captured Raman intensities and the repetition rate can be confirmed within the presented measurements. This result is shown exemplarily for the Raman peak with the largest intensity

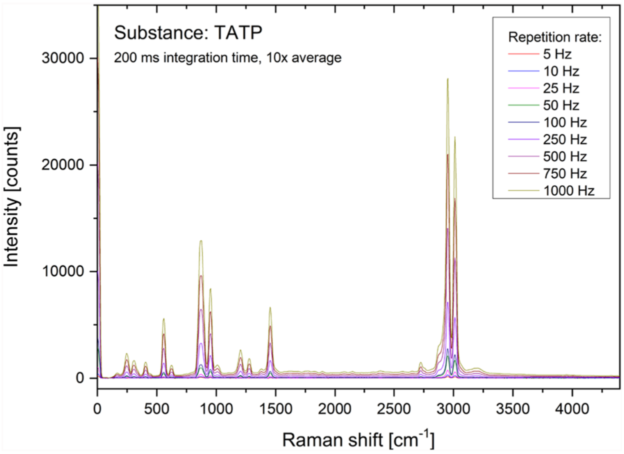


Fig. 2 Raman spectra of the explosive substance TATP collected at different laser pulse repetition rates and with a spectrometer integration time of 200 ms, calculating an average over 10 single spectra

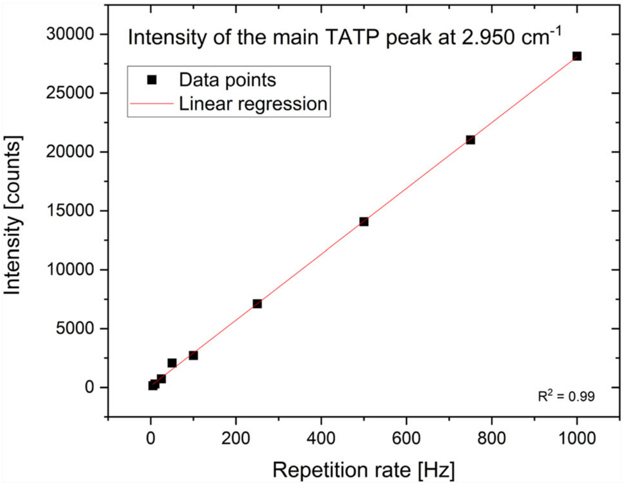


Fig. 3 Illustration of the observed linear dependency between the intensity of the strongest raman peak of TATP (2.950 cm-1) and the laser pulse repetition rate

at 2.950 cm^{-1} in Fig. 3. After performing the Raman analysis, all TATP samples are irradiated with the cw laser with sequential increasing average optical power. As a result, it can be proven that the samples can easily be ignited during the irradiation with a continuous-wave laser with sufficient optical power. In comparison, the pulsed laser source with the same wavelength can safely interact with the TATP sample even at the highest checked repetition rate of 1000 Hz. For example, samples that could securely be irradiated with the pulsed laser system at a power density of over 95 W/cm^2 showed on the other hand ignition effects with the continuous-wave laser even at lower values around 32 W/cm^2.

Figure 4 shows Raman spectra of different samples of black powder. Black powder hereby is technically defined as a mixture of sulphur, charcoal and potassium nitrate. The spectrum of a single black powder grain (~ 5 mm diameter) is shown in comparison with fine black powder with smaller particles in the micron range. It can be stated that there is no difference in the spectral signal and again that the Raman signal gets stronger with increasing repetition rate, leading to more pulses interacting with the sample during the same time. For the measurement of black powder, the integration time of the spectrometer has to be increased to 500 ms, and it is necessary to average over more single spectra for a smooth spectrum.

Further experiments are carried out with mixtures of black powder and TATP in different percentage weight ratios. In case of mixtures, combined Raman spectra of both substances can be collected like exemplarily shown in Fig. 5 for a mixed sample of 90% TATP and 10% black powder. The comparison of the spectral data shows that the mixed spectrum contains all significant peaks of TATP and also additional peaks that can be assigned to the black powder admixture. As a drawback, it must be stated that the signal strength for the Raman measurement of black powder is significant weaker than for TATP when it comes to otherwise similar measurement parameters. This is consistent with reports from the literature that also show challenging conditions in case of black powder as a target substance, leading to the necessity of longer measurement times or higher laser intensities [11]. During the ignition experiments, all black powder samples and also the mixtures of TATP and black powder proved their ignitability with continuous-wave (cw) laser irradiation, whilst none of the experiments with the nanosecond pulsed laser showed any ignition of the substances at all. Mixtures of black powder and TATP showed a more critical ignitibility than the pure substances. For the specific ignition mechanisms, different assumptions and models are stated in the literature. The energy transferred directly to the explosive by the laser radiation leads to ignition when a critical material-specific threshold is exceeded. A large number of influencing parameters such

Fig. 4 Comparison of raman spectra of different samples of black powder with two different laser pulse repetition rates (500 Hz and 1000 Hz)

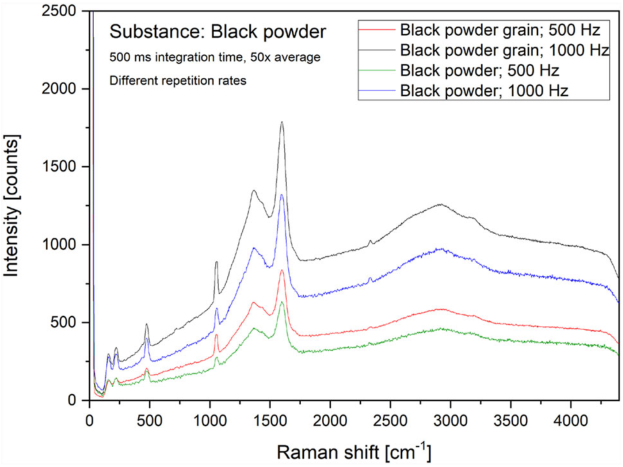
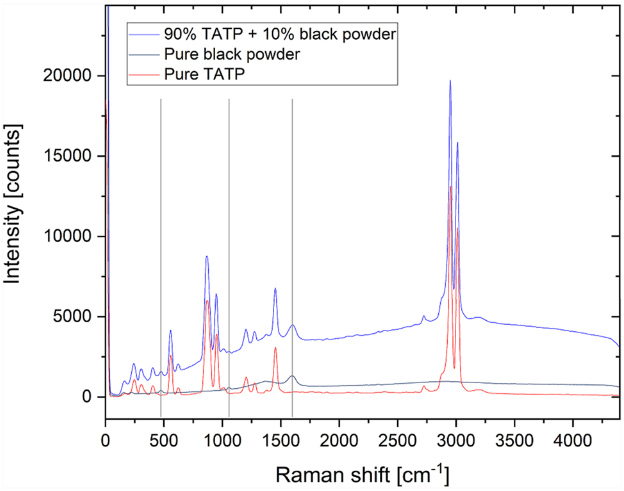


Fig. 5 Comparison of raman spectra of pure TATP, pure black powder and a mixture of both with 90% TATP and 10% black powder (percentage by weight)



as laser wavelength, repetition rate and power density as well as the irradiated volume in the material play a role here [12]. Longer pulse durations also lead to lower ignition thresholds, which indicates the involvement of thermal ignition mechanisms, whereby the heat conduction properties of the explosives are important. The ignition of the energetic material starts with the formation of so-called hot spots at inhomogeneities in the material. If a specific energy threshold is exceeded, the number of hot spots is greatly increased, which ultimately results in ignition [13]. Local temperatures of over 700 K and hotspot lifetimes of longer than 10 µs can be understood as critical [12].

Measurements under more realistic conditions with the influence of ambient light during the measurement show that it is still possible to analyse the substance after performing a background correction algorithm on the spectral data. This is exemplarily shown for TATP and with a repetition rate of 25 Hz in Fig. 6. The background correction method is performed by fitting a spline function to the spectral data with specific chosen support points. The spline curve is then subtracted point by point from the measured spectral data, leading to an analysable spectrum. As a drawback, it must be stated that the intensity is weaker than the original spectral data measured against blocked ambient light.

Further efforts are undertaken to transform the first laboratory set-up to a miniaturized version. This new set-up consists of the laser source and the spectrometer (*Flame, Ocean Insight*) both directly attached to a small optomechanical cube. This cube contains all necessary optics and provides an output window pointed to the analysed substance. The working distance in this case is chosen to be 1–2 cm. The direct attachment of the spectrometer eliminates the necessity of a glass fibre, and with the direct placement of the laser, no long open-path lengths are used in this compact set-up. A photograph of the final compact and miniaturized set-up is shown in Fig. 7. While this set-up is designed to be brought to use in close distance to the analysed substances, one can imagine improvements in terms of stand-off capabilities. This could be accomplished by implementing a new optical unit consisting a telescope and other beam forming elements in order to achieve a defined laser interaction with a target substance over longer distances and the ability to collect a significant amount of Raman signal coming back from the target. As a drawback, it can be stated that this design would exceed the compactness of the suggested set-up and could prevent the possibility of a handheld or portable solution.

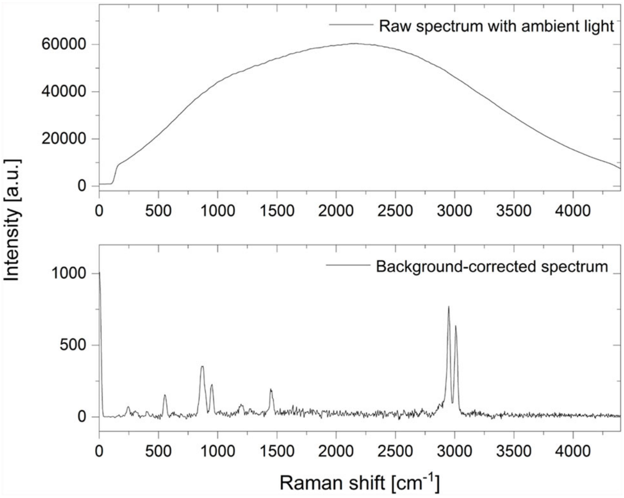


Fig. 6 Exemplarily demonstration of a background-corrected spectrum of TATP measured in a realistic setup with the influence of ambient light

Fig. 7 Photo of the final miniaturized laboratory setup consisting a small optomechanical cube (30 mm cage system) with directly attached laser source *(FDSS 532-Q4, Crylas GmbH)* and compact spectrometer *(Flame, Ocean Insight)*

4 Conclusions

In this work, it can be shown that it is possible to collect Raman spectra of good quality in short measurement times without any observed ignition of different relevant sensitive explosives. Even for mixtures of black powder and TATP which are particularly critical in terms of their ignitability, it can be successfully demonstrated. This is achieved by using a pulsed nanosecond laser at a wavelength of 532 nm with suitable laser parameters. A direct comparison with a continuous-wave laser of the same wavelength shows that all irradiated explosives can be ignited in principal. In the case of substance mixtures, it is possible to record Raman lines of both substances in a combined spectrum. For black powder samples, the measurement time has to be significantly extended compared to the measurement of TATP, but still lying within an acceptable range for the applicational needs. Realistic measurements under the influence of ambient light show that the impact can be significantly reduced with the use of suitable data evaluation methods, so that an analysis of the Raman spectra is also achievable in this case.

Further steps are undertaken to minimize the experimental set-up, especially by redesigning the optical unit and by attaching it directly to the laser source. With the spectrometer coupled directly to the set-up, there is no need for connecting glass fibre. Future plans are to build up a database with more substances and further integrate all components to a portable prototype.

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Data Availability The manuscript has associated data in a data repository

Declarations

Conflicts of interest The authors declare no conflict of interest.

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