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An Approach to Reduce the Sample Consumption for LIBS based Identification of Explosive Materials

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ABSTRACT

An experimental design based on spectral construction, which has potential to minimise the sample consumption, the number of laser shots and time required to collect the data from laser induced breakdown spectroscopy for identification of the explosive materials is reported in the study. This approach is an ideal solution in the field of hazardous material detection, where the availability of the sample can be a serious limiting factor. The experimental data recorded on a set of five high energy materials has been considered to test the performance of the proposed methodology. Multiple spectra are constructed by assuming a normal distribution at each wavelength of the spectrum, where random numbers are generated using the mean and standard deviations obtained from arbitrarily chosen five experimental spectra from each class. The newly generated spectra are called as synthetic spectra. The correct classification obtained from – K - nearest neighbour combined with principal component analysis and partial least square – discriminant analysis demonstrated very promising results. The correct classification rates differed by only 4 per cent - 7 per cent as compared to conventional approach where experimental spectra alone are considered for the analysis. Further, when RDX is excluded, the obtained results are almost identical with conventional approach.

Keywords: Laser induced breakdown spectroscopy; Synthetic spectra; Identification; K – Nearest neighbour

1. INTRODUCTION

Laser induced breakdown spectroscopy (LIBS) employs a laser pulse to create a plasma source that emits light in the visible and near infrared regions[1-3]. The emission strength depends on various parameters including the number of emitting species, plasma temperature[4], matrices on which the sample is present[5] and the environmental conditions. The possibility of stand-off/remote detection, minimal sample preparation and capability of getting the signal from all the elements of the periodic table are great advantages and make it an attractive spectroscopic tool. LIBS spectra can be used in two distinct ways - elemental analysis[6,7] and material classification/identification[3,8]. While the elemental analysis utilises calibration[9], calibration –free[10,11] or multivariate methods[12], classification/identification relies predominantly on the multivariate methods[3,12]. LIBS has added a new paradigm in various fields like space[13], archaeology[14], biology[15], isomer identification[16] biomedical[17,18], industrial[19], defense[2,20], food processing[21], nuclear waste[22] and forensics[23, 24]. LIBS received a boost with the availability of the compact, high power lasers and Echelle type gratings for the applications related to classification and identification of materials. There is a growing interest towards LIBS as a potential technique for the detection of high energy materials (HEMs) because of its stand-off capability[25]. LIBS is also incorporated on Mars rover curiosity with a measurement distance of seven meters[26].

Detection of HEMs with LIBS poses several challenges, such as similar elemental composition of Carbon (C), Hydrogen (H), Oxygen (O) and Nitrogen (N), the common interferences like grease, oils, biological material[27], etc. In addition, the presence of oxygen, nitrogen in the ambient air and hydrogen, oxygen in moisture can be a serious problem for field experiments. It has been demonstrated that with the application of various chemometric algorithms, it is possible to distinguish the similar type of materials based on their LIBS spectra. Different methods like soft independent modelling of class analogy (SIMCA)[3], partial least squares –discriminate analysis (PLS-DA)[28,29], support vector machines (SVM)[30, 31] and artificial neural networks (ANN)[32,33] etc. have been successfully implemented for the classification of a wide variety of materials. In this approach, multiple spectra are recorded to incorporate all possible variations that can arise with the type of system in use. As a next step, these datasets are used to create a model and test the identification capability. However, there are few limitations while recording the multiple data sets –

(a) Sufficient number of data sets for accurate representation of the possible variations is not clear
(b) Availability of sufficient quantity of sample for recording multiple datasets
(c) Time required to record the data.

In this paper, authors investigated the feasibility of a novel methodology to construct multiple spectra using a very small number of experimental spectra. This approach eliminates the need of acquiring a large number of experimental spectra. It is now possible to generate a required number of spectra which

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otherwise may be impractical to acquire experimentally. This can greatly reduce the load on the resources in terms of laser shots and time taken for the experiments. Finally, validation has been done using two different classifiers, PLS-DA and KNN.

2. MATERIALS AND METHODS

2.1 Experimental

The samples were irradiated by the pulses from the second harmonic of Nd: YAG laser at 532 nm, 7 ns at 1 Hz[34]. The details of the experimental setup can be found in Myakalwar[35], *et al.* Experiments were performed on a set of five HEMs- HMX, NTO, PETN, RDX, and TNT in ambient conditions to acquire multiple spectra. As KNN requires the same size of dataset of each class, sixty spectra per sample were considered.

Typical LIBS spectra of all samples normalised to oxygen peak centred at 777.2 nm are as shown in Fig. 1[35]. Each spectrum is constituted with 25699 data points. The obtained spectra have features of C, Mg, Ca, H, N, O, Na, CN and C_2. The Oxygen peak at 777.2 nm is dominant followed by CN at 383.3 nm. CN and C_2 peaks are the characteristics of organic molecules.

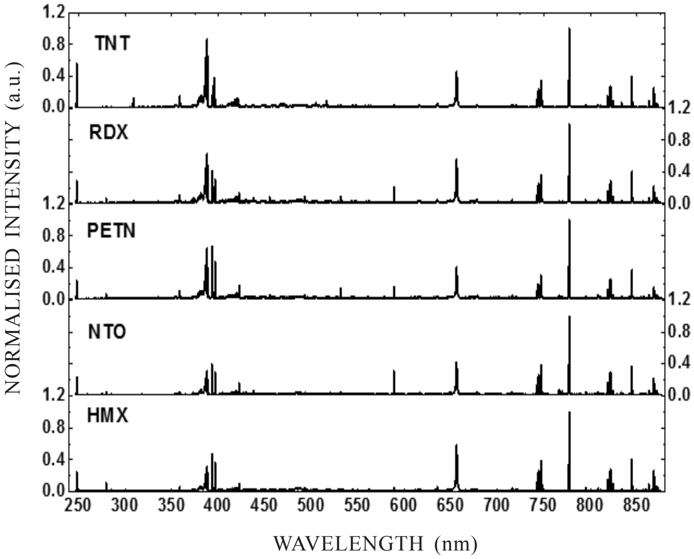

Figure 1. The typical LIBS spectra of TNT, RDX, PETN, NTO, and HMX normalised to Oxygen peak centered at 777.2 nm.

Although the spectra of all the classes are almost identical, the peak intensities exhibit variations among and within the classes. The fluctuations among the spectra of the same class may be attributed to different reasons like the uncertainty in laser energy and inhomogeneity in the sample morphology. The mean and standard deviation(s) at each wavelength are the key features for constructing multiple spectra. The fluctuations are modelled with a normal distribution as inferred from the quintile - quintile plot. The details of the methodology will be explained in section 3. K – Nearest neighbour combined[36,37] with principal component analysis and partial least squares –discriminate analysis have been employed for validating the proposed methodology.

2.2 Methodology

The conventional way of identification of materials involves the acquiring multiple spectra per class from the LIBS experiment. These spectra are utilised for training, validation and testing the model. The method investigated in this paper uses only a very small number of experimental spectra. After acquiring the spectra, there are two steps in this approach

(a) Construction of spectra with the aid of a little number of experimental spectra and
(b) Multivariate analysis to obtain the percentage correct classification.

The intensities at a given wavelength of the experimental spectra is modelled as a normal distribution with the probability distribution function given by,

$$F(I_\lambda) = \frac{1}{\sigma_\lambda\sqrt{2\pi}} e^{\frac{-(I_\lambda - \mu_\lambda)}{2\sigma_\lambda^2}}$$

where σ_λ, μ_λ, and I_λ corresponds to standard deviation, mean and intensity count at each wavelength respectively. The mean and standard deviation(s) are calculated at all wavelengths for each class of the experimental spectra. The intensity at each wavelength varies from one spectrum to another in accordance with the distribution stated above. These parameters are specific to each of the samples considered. The construction of spectra is performed by generating random numbers for each wavelength using mean and standard deviation(s) obtained from the experimental spectra. These constructed spectra are called as synthetic spectra.

The second part of the methodology involves the process of building a chemometric model which is capable of identifying an unknown test sample. A chemometric model is constructed based on a data subset which is referred to as a training set. As a next step, the model is tested using the remaining part of the data which is referred to as testing set. The analysis is performed to mimic the actual application scenario where synthetic spectra are used for training and testing is performed on the experimental data. The results are compared with the traditional method, where both training and testing are performed on only the experimental data. The efficiency of detection can be quantified in different ways, one of such parameters is the percentage correct classification (PCC). The data has been split into training, testing sets multiple times and the correct classification is taken as an average over multiple iterations. The flow chart of complete algorithm is as shown in Fig. 2.

3 RESULTS AND DISCUSSIONS

The mean and standard deviation(s) were calculated at each wavelength of the full spectrum for all the five classes separately for randomly selected five experimental spectra. The number of experimental spectra that need to be considered has been estimated on the basis of fluctuations in the mean and standard deviation(s). A typical graph of mean and standard deviation(s) with error bars calculated from hundred iterations and relative standard deviation at 247.8 nm (Carbon) for HMX is as shown in Figs. 3(a) and 3(b). It can be seen from Fig. 3, that the mean and standard deviations does not show a considerable variations for a number of spectra more than five.

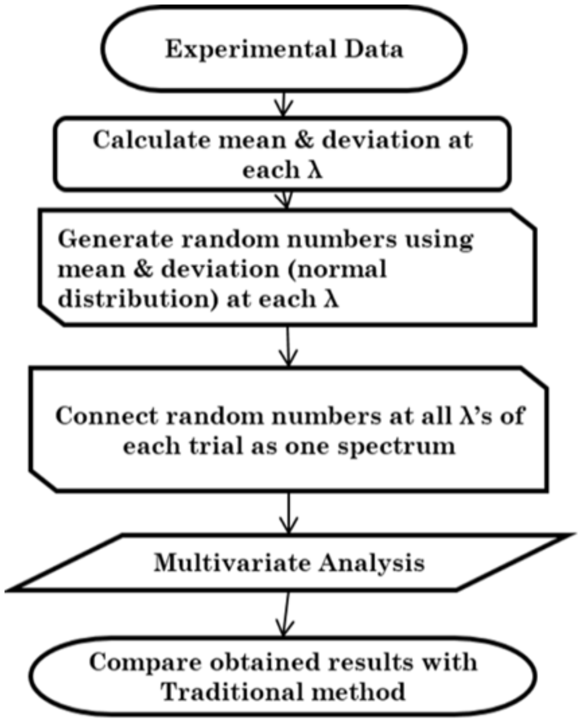

Figure 2. The flow chart of steps involved in proposed method.

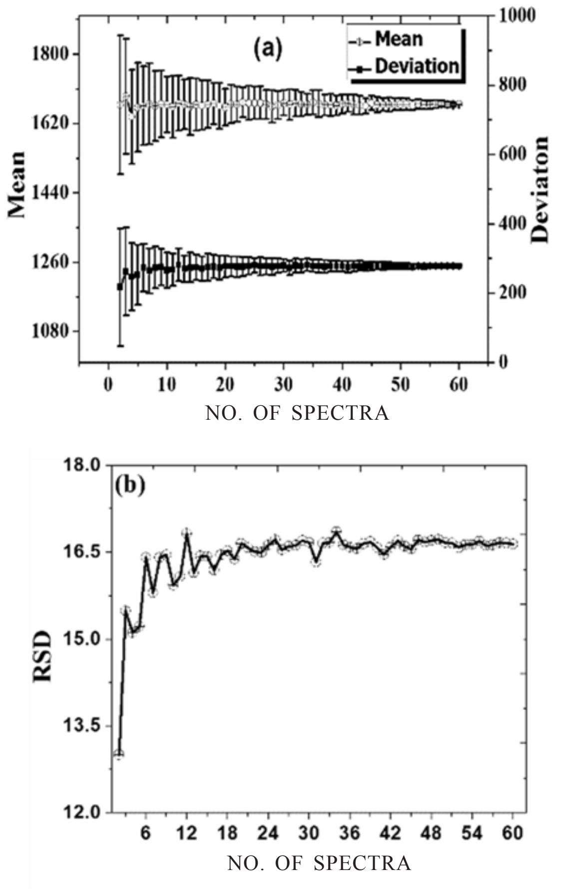

Figure 3. (a) The mean (top) and standard deviation (bottom) with error bars calculated over 100 iterations and (b) Relative standard deviation, as a function of number of experimental spectra for HMX at carbon peak 247.8 nm.

Sixty random numbers were generated in normal distribution at each wavelength for each class separately, using the mean and standard deviation(s) of five experimental spectra. A typical synthetic spectrum was constructed, by connecting the generated random numbers at all wavelengths in a single trial. These spectra were smoothened by multiscale principal component analysis to nullify the undesirable randomness introduced in the synthetic spectra especially at peak positions. A typical normalised synthetic spectrum together with an experimental spectrum is as shown in Fig. 4(a). The overwhelming similarity between the synthetic and the experimental spectra is evident. Figure 4(b) shows the dendrogram with experimental and synthetic spectra. The leaves of a single clade in a dendrogram clearly belong to a single class.

At this point, there are two sets of data – experimental and synthetic. Each set consists of sixty spectra per class which imply three hundred spectra per set. Two classifiers

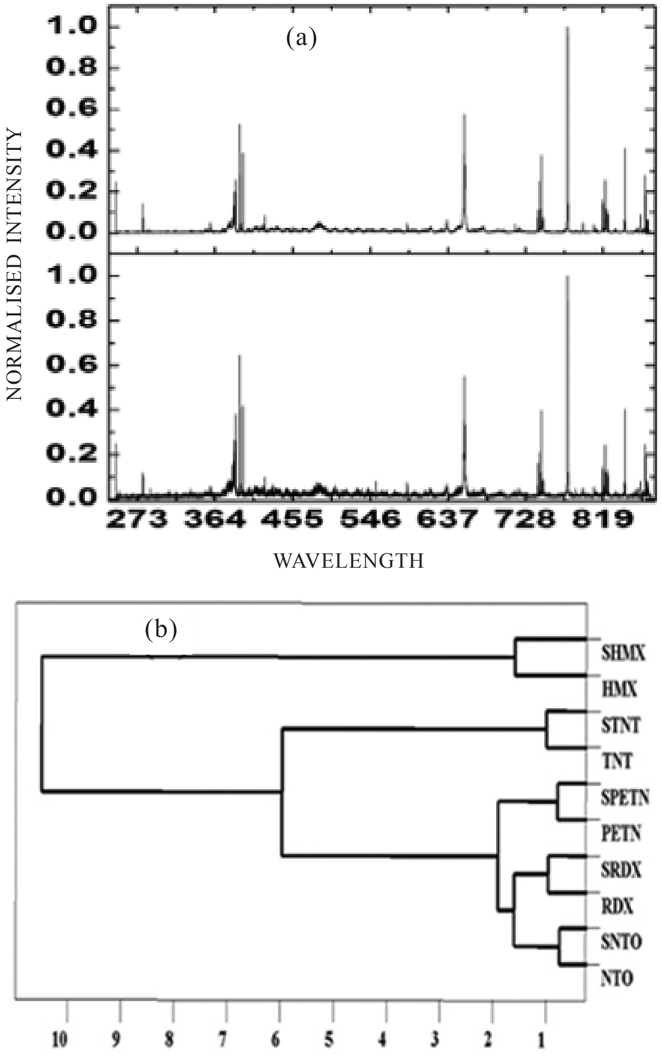

Figure 4. (a) A typical LIBS spectrum of experimental (bottom) and synthetic (top) for HMX normalised to OI centered at (777.2 nm) peak and (b) The dendrogram representation of experimental and synthetic spectra for five samples. The prefix 'S' stands for synthetic.

KNN-PCA and PLS-DA have been employed for estimating classification efficiencies. The analysis performed for only the experimental set will be referred to as the traditional method. The experimental data has been split into training and testing sets of 70 per cent and 30 per cent respectively. In the proposed method, the training was performed by choosing 70 per cent of the synthetic spectra and testing was done with 30 per cent of experimental data to mimic the practical scenario.

Since PCA is an unsupervised technique, KNN is performed after executing the dimensionality reduction with PCA for quantification. Here the features are the first three principal components (PC's) extracted from the given data using PCA. Similarly, the test data set was also projected onto PC space. Optimisation of K- parameter has been done in each iteration with a validating data set, by considering K value at maximum PCC. Typically, its value was one to eight for experimental data and one to three for synthetic data**.** In the case of PLS-DA, the number of PLS components were fixed at five for simplifying algorithm. The averaged PCC for all sample classes are as shown in Table 1. The PCC's were averaged over hundred iterations, wherein each time training and testing sets were randomly selected. It can be seen, except for RDX, the PCC with the proposed method shows an excellent agreement with the traditional method.

Table 1. Comparison, of the PCC obtained with the proposed method for five classes of samples with KNN-PCA and PLS-DA with the traditional method

PCC	KNN-PCA		PLS-DA	
	Traditional	Proposed	Traditional	Proposed
HMX	100.00	100.00	88.89	100.00
NTO	100.00	100.00	100.00	94.44
PETN	98.11	93.11	100.00	94.44
RDX	95.22	63.22	83.33	61.11
TNT	100.00	100.00	100.00	100.00
Average	98.66	91.26	94.44	90.00

HMX, NTO and TNT have not shown any mis-classifications with both the traditional as well as the proposed methods with KNN. But in the case of RDX, the mis-classification rate was very high about ~ 37 per cent with the proposed method. One possible reason for this peculiar behaviour could be due to the high fluctuations in the experimental RDX spectra (testing data set) as it was very difficult to keep RDX pellet intact. The pellet was very delicate and broken while acquiring spectra. However, more detailed experiments need to be performed to ascertain the reasons.

Here in RDX has been mis-classified as either PETN or NTO with KNN or as HMX with PLSDA. However, if the RDX is omitted from the average, the proposed method shows identical results as compared to the traditional method. In view of the standard deviation of 2 per cent - 3 per cent in PCC, the results can be considered as identical. Though the PCC with five samples included was less than the traditional approach, it is important to note that the difference is only about 4 per cent - 7 per cent with only five experimental spectra used. Considering the fact that only five experimental spectra were utilised for the analysis, and the classification rates of above 90 per cent are very encouraging. The PCC were calculated as a function of the number of synthetic spectra. Here, a different number of synthetic spectra were generated and the same protocol was used. The results showed no significant dependence on the number of synthetic spectra.

The results show that the synthetic spectra based method can substitute the traditional methodology for dealing with classification and identification problems using LIBS data. It is important to note that while in the traditional method sixty experimental spectra per class were used whereas in the proposed method only five experimental spectra per class were used. The results have multiple implications on how the experiments for classification related applications can be performed with very limited quantity of sample, resulting in reduction of time required to perform the experiment and most importantly reduction in the number of laser shots. The reduction in the number of laser shots can enhance the life time of a laser, which will be of considerable interest for a field device operated on a battery.

4. CONCLUSIONS

A novel spectral construction method for LIBS based explosive classification/identification has been studied. We successfully showed that this approach has the potential to drastically reduce the sample consumption for performing LIBS experiments, by eliminating the need of experimental repetition. The average percentage correct classification shows an excellent agreement with the traditional method. This method can result in overall reduction resource investment for performing LIBS based classification/identification experiment. It may be generalised and adapted to deal with similar kind of problems employing other spectroscopic methods.

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He has conceived the idea presented in this paper, planned and assisted in writing the manuscript.