Seminar

Institute for Plasma Research

Title : Study of Laser Induced Plasma Spectroscopy coupled with machine learning methods for various analytical applications

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Venue : Online - Join the talk:
https://meet.ipr.res.in/Dr.PraveenDevangad_PDFTalk

Abstract :

Atomic emission spectrum obtained from laser produced plasma is an important source to investigate the composition of the material. This spectrum consists of large number of atomic and ionic lines/signatures which are unique for every element present in the given sample/material. The study of such emission features in a weakly ionized plasma is popularly known as Laser Induced Plasma Spectroscopy. This method is fast, cost effective and has multi-elemental detection capabilities. Being quasi non-destructive method, the spectrochemical analysis of soilds, liquids as well as gases can be carried out. The interaction of Q-switched, nanosecond Nd:YAG laser of few milli Joule of energy is focused on a sample to produce the spectrum. The plasma is collected and sent to the spectrograph to record the spectrum.

The ultimate goal of an analyst is to identify the class of material, or to determine the amount of analyte present in it with fairly good accuracy and precision. However, to meet these requirements one has to investigate the following challenges of Laser Induced Plasma Spectroscopy. (1) The spectrum is complex due to the laser matter interactions, ambient conditions and sample inhomogeneities. This causes the issues of reproducibility and overlapping of emission lines in the spectrum. (2) Further, high-resolution echelle spectrographs can generate the data from 200 nm to 850 nm which consists hundreds of emission lines of respective elements. In other words, every analyte has multiple (tens to hundreds) emission lines and hence the spectrum is multivariate in nature. To address these challenges machine learning (multivariate) methods have been implemented for the analysis of glass samples. Glasses are considered as a complex material due to large number of elements present in it. Calibration curves were constructed using partial least squares (PLS) to analyse the prototype nuclear waste (borosilicate glass) materials. The results obtained from PLS outperformed the traditionally used univariate method. Similarly, Sr, Cr and Ti doped iron phosphate glasses were synthesized and their spectra were analysed using support vector machines (SVM) along with PLS methods. Regression curves obtained from SVM method found to be better than PLS for certain analytes. The figures of merit were presented in the form of correlation coefficient (R^2), root mean square error of calibration (RMSEC) and root mean square error of cross validation (RMSECV). Additionally, the classification of glass materials was also performed using principal component analysis (PCA), partial least square discriminant analysis (PLS-DA) and SVMs. The performance of the method is discussed in terms of sensitivity, specificity and accuracy.

We have successfully demonstrated the efficacy of machine learning methods to analyze the spectra of laser produced plasma. Similarly, we can extend this work for any other complex samples/materials.

Keywords: LIBS, Glass, Machine learning methods, Quantification, Classification