Indigenous development of automated cost-effective system for SERS measurements with data analysis and compound prediction

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Surface enhanced Raman scattering (SERS) process enhances the Raman signal of various analytes in presence of plasmonic gold and silver nanoparticles [1]. SERS finds applications for compound identification in various fields like food safety, narcotics, explosive detection, bio-medical etc. Inspite of significant signal enhancement in SERS, its popularity in real-life applications is still scanty due to variation in Raman signal both intensity and pattern, with respect to type of SERS substrate, laser excitation wavelength and detector type, and also limited methodologies for accurate prediction of compound mixtures. Recently, advancement of data analysis methods like machine learning (ML) and deep learning (DL) are shown to be useful for accurate compound predictions from SERS data [2]. The results predicted from ML/DL methods are more accurate when the training dataset consists of different possible variations in spectral data of a given compound or mixture. However, such datasets are not available in public domain and these have to be produced experimentally. Further pre-processing i.e. background and noise removal of large data sets with visualization of individual spectra makes the process cumbersome. This necessitates requirement of a high-throughput system for faster and automated measurement of large number of samples with quick data processing and analysis.

In this regard, we have indigenously developed a completely automated cost-effective system for Raman and SERS measurements with data-analysis and machine learning based compound prediction. The system consists of in-house developed computer controlled low-cost XYZ translation stage using Arduino and CNC shield for sample movement and in-situ sample viewing using low-cost USB microscopes and Raspberry Pi based computer. The translation stage helps for automatic measurement of multiple samples and sample-viewing system helps monitoring the location of measurement and stand-off distance. These two hardware modules are integrated with a portable Raman spectrometer through automation software written in Java Script, React and Python. The user has to mention the input parameters like number of samples with location matrix and multiple integration time of measurements. Without human intervention, the system can take all measurements and save the files with auto-naming using measurement details. After the measurements, automatically the data processing software activates the pre-processing of measured data and performs different ML based compound classification of the measured samples. Fig. 1(a) and (b) present a schematic lay-out of different hardware and software modules and photograph of the developed system respectively.

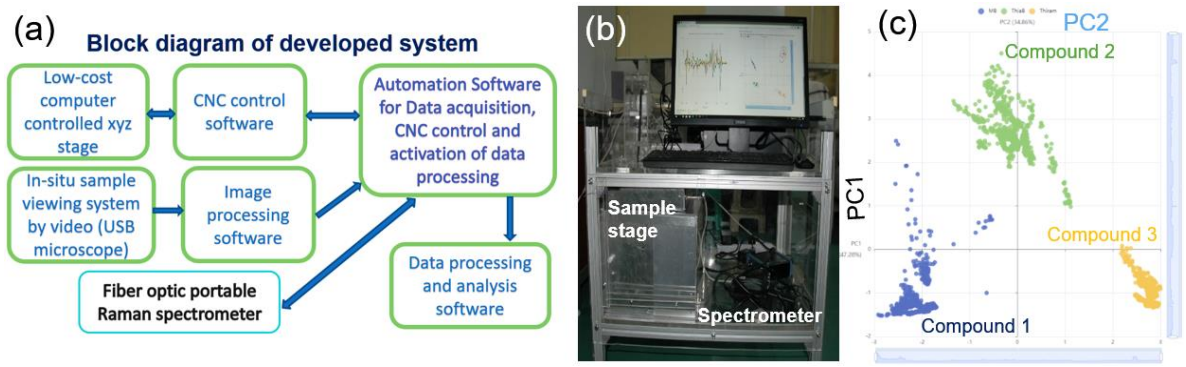

Fig. 1(a) System block diagram of hardware and software modules, (b) photograph of the developed system and (c) view of PCA based compound classification

The developed system significantly decreased the workflow time. It was tested to acquire 1000 spectra (5-10 s integration time) with subsequent pre-processing and principle component analysis (Fig.1c) within 5 hrs. The system is useful for R&D users for quick comparison of performance of different ML models for compound classification and determines need of DL model for prediction with higher accuracy. It is unique system designed with low-cost hardware and integrates different in-house developed software, which is upgradable as per end user requirements. It is also beneficial for industrial users requiring rapid analysis of large number of samples on regular basis like raw material verification, process monitoring, quality control of products etc.

References

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