A Composite Algorithm for Optimized Baseline Correction in Raman Spectroscopy

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Abstract: We propose a novel algorithm for the pre-treatment and recovery of Raman signals from fluorescence contaminated spectra. This algorithm combines the second derivative and iterative smoothening routines for optimized spectral baseline estimation and correction.
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1. Introduction

Fluorescence contamination, observed as backgrounds surmounting relatively tiny Raman peaks in a spectrum, is a well acknowledged nuisance in Raman spectroscopy [1-3]. This have led to the development of several procedures for pre-treating Raman signals prior to any meaningful analysis [1, 2]. These procedures employ specialized instrumentations and/or computational methods to recover embedded Raman signals. Computational methods are however, much more preferred because they are cost effective, convenient for portable systems and can be automated.

The computational methods involve the application of predefined mathematical algorithm on a measured raw spectrum data to estimate and subtract the baseline. Two outstanding predefined mathematical algorithms widely employed for this purpose are the second derivative method [1] and the iterative smoothening method [3].

The second derivative method is able to eliminate the spectral baseline and reveal hidden peaks. However, it introduces side bands which hampers spectral matching and interpretation. The smoothening methods, on the other hand, are able to effectively determine and remove underlying spectral baselines leaving only the pure Raman signals. But, the processes adopted for determining appropriate criteria for convergence in the iterative methods are subjective.

In this work, we have developed a more resolute algorithm that combines the second derivative and iterative smoothing methods, which is very efficient in pre-treatment and recovery of Raman signals from fluorescence contaminated spectra.

2. Theory and Algorithm Description

A measured spectrum $(S(v))$ consisting of pure Raman signals $(R(v))$ and Fluorescence contamination (L) is expressed mathematically as $S(v) = R(v) + L$. The second derivative of $S(v)$ eliminates the fluorescence term leaving the Raman signal in its derivative form as

$$d^2R(v)/dv^2 = 8a_0(v-a_1)^2/a_2^4(1+(v-a_1/a_2)^2)^3 - 2a_0/a_2^2(1+(v-a_1/a_2)^2)^3 \qquad (1)$$

where a_0 , a_1 and a_2 are the amplitude, center position and width parameters of the Raman peaks respectively considered as Lorentzian function. The iterative smoothening process is described with the flowchart in Fig.1.

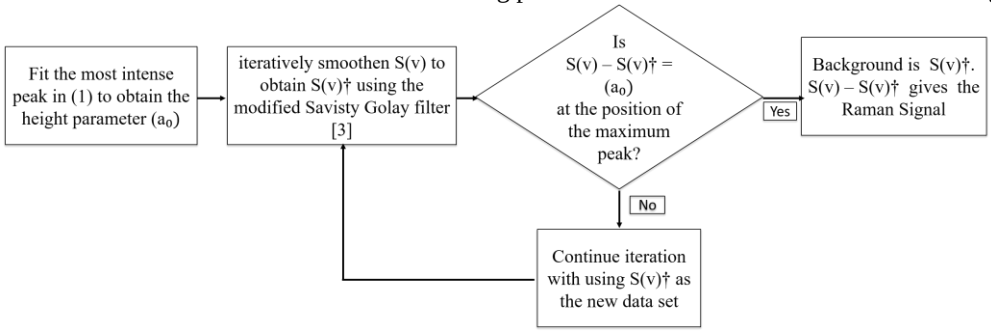

Fig.1. flow chat decribing the iteratve process of the agorithm

3. Simulation and Application Results

Fig. 2. Illustrates the procedure of our method with contaminated. Results obtained by applying this method on experimentally measured Raman spectra of Glucose (Fig. 3. A) and Sulphur (Fig. 3. B) have been demonstrated.

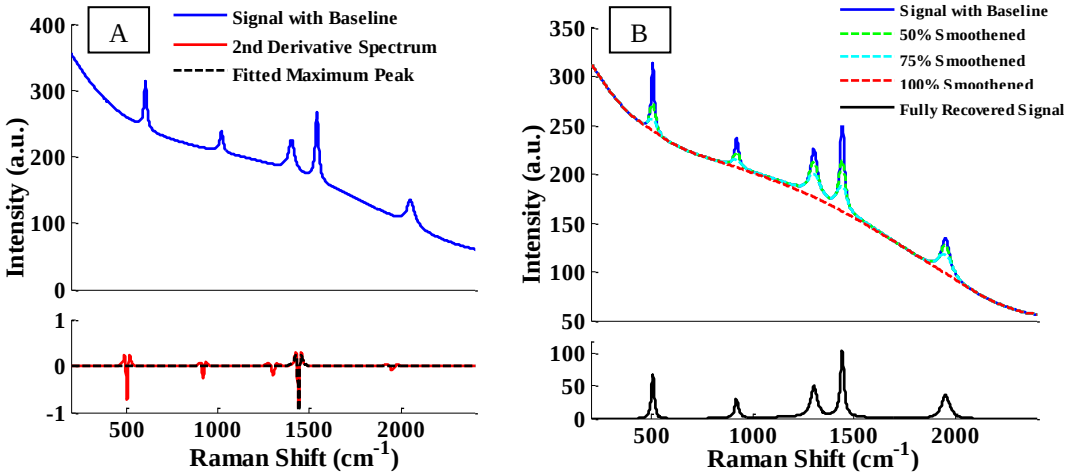

Fig. 2. (A) is the contaminated Raman spectra and its second derivative with the most intense peak fitted and (B) Shows the various stages of the smoothening until the amplitude of the most intense peak has been recovered

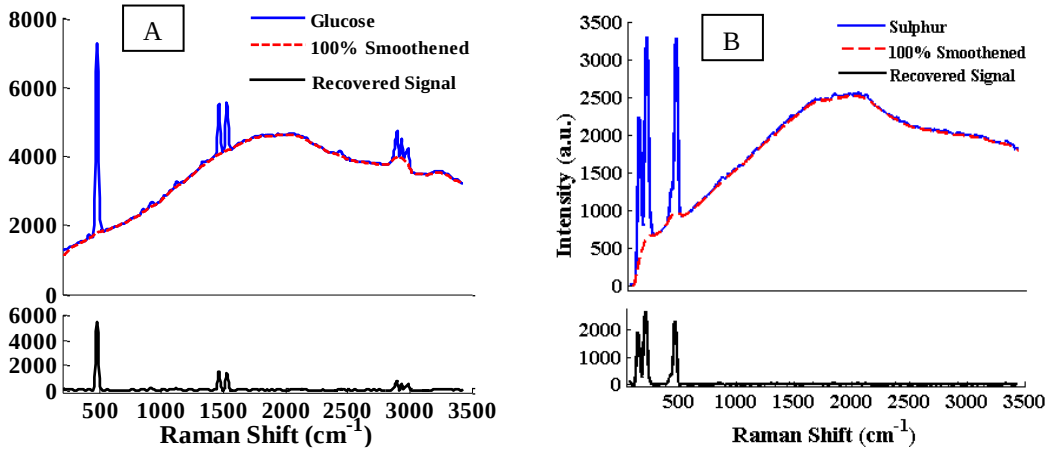

Fig.3. Application results of the proposed method for (A) Glucose and (B) Sulphur

4. Conclusions and Further work

An objective algorithm has been developed by combining second derivative and iterative smoothening methods for pre-treating Raman spectra embedded in fluorescence contaminated spectra.

5. Acknowledgements

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6. References

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