Removing Background of Raman Spectrum Based on Wavelet Transform

Gang Li
Faculty of Mechanical and Electronic Information
China University of Geosciences
Wuhan, 430074, China
ligang_chn@yahoo.com.cn

Abstract—**Raman spectrum is usually so weak that the noise usually distorts the interesting Raman bands. Especially, when the sample is fuscous, the strong fluorescence background often completely dominates Raman peaks. In this case, it is vital to remove fluorescence background for analyzing of Raman spectrum. Wavelet transform (WT) has proved to be a high-performance signal processing tool, and very efficient in removing low frequence noise. In this paper, WT was used to remove fluorescent background of Raman spectrum of Sudan I. Both the global thresholding method and the interval thresholding method were applied, and their de-noising performances were compared. The results indicated that the interval thresholding method is more efficient than the global thresholding method in removing fluorescence background of Raman spectrum.**

Keywords- Raman spectrum; wavelet transform; fluorescent background; noise removal

I. INTRODUCTION

A. Raman specroscopy

As a technique with multiple disciplines intercrossing and syncretizing each other, Raman spectroscopy is on its developing time now, and studies on its applications are being on the way to advance. Now Raman spectroscopy has becoming an effective analysis tool [1, 2], and been used more and more widely because of its' convenient, powerful and non-destructive advantages. However, the Raman spectrum is usually very weak, so that the noise usually distorts the interesting Raman bands. When the sample is fuscous, the strong fluorescence signal often completely dominates the weak Raman peaks. In this case, it is vital to remove fluorescence background from Raman spectrum for qualitative and quantitative analyses of Raman spectrum.

B. Wavelet transform

Wavelet transform (WT) has proved to be a high-performance signal processing tool [3, 4], and very efficient in de-noising. Mittermayr, Nikolov, Hunter and Grasserbauer used several de-noising methods of WT to de-noise the noisy signals, compared their performances, and their results indicated that the WT method is more satisfactory than classical methods [5]. Now, WT has been widely employed to remove both low frequence and high frequence noise [6-8].

When WT is used to de-noise a signal, the thresholding method is very important to the reconstructed signal. The hard and soft thresholding are two main methods for compressing wavelet coefficients. An improved method, block thresholding, has been proposed [9]. The procedure divides the coefficients into blocks, and then makes simultaneous decisions to retain or discard all the coefficients within a block. The utilization of information about neighboring wavelet coefficients increases the estimation precision. The method has been applied to de-noise Raman spectra [10]. About the selection of thresholds, several methods have been studied. The standard methods include the level-dependent and interval-dependent threshold selections. The level thresholding method selects one universal threshold for each level, and uses it to threshold all the coefficients at the level. The interval thresholding method first divides the coefficients at each level into blocks, and then selects a local threshold for each interval to threshold the coefficients within the interval. They are both widely used to de-noise Raman spectra [10], but few studies have focused on comparing their performances of de-noising fluorescent background of Raman spectra.

II. DE-NOISING THEORY AND METHOD OF WT

Using WT, the time and frequency characteristics of the signal are captured, and the obtained approximation and detail coefficients respectively represent the low and high frequency components of the analyzed signal. Because fluorescent is mainly composed of low frequency components, the background removal is performed by thresholding the approximation coefficients.

Removing fluorescent background procedure usually involves three steps. Firstly, the noisy signal is transformed into a set of orthonormal wavelet basis functions. Secondly, threshold values and thresholding method are applied to compress the approximation coefficients. And then the thresholded coefficients are assembled back to obtain the signal without the noise.

III. EXPERIMENTAL

The Raman spectrum of Sudan I was obtained in Raman System R-3000 spectrometer manufactured by Boston

978-0-7695-3676-7/09 $26.00 © 2009 IEEE
DOI 10.1109/FCC.2009.69

Advanced Technologies (Marlboro, MA, USA). The instrument uses an Ocean Optics S2000 spectrometer as the monochromator, which uses an uncooled 2048-element linear silicon CCD array to measure spectra from 0 cm^{-1} to 2700 cm^{-1}, and has a spectral resolution of about 10 cm^{-1}.

Sudan I of 95% purity and analytical grade was provided by No.3 Branch of Shanghai Chemical Reagent Company (Shanghai, China). Raman spectrum of Sudan I was measured under about 22°C temperature.

IV. RESULTS AND DISCUSSION

A. Selecting level of decomposition

Raman spectrum of Sudan I was decomposed using db4 wavelet. Fig. 1 showed experimental Raman spectrum of Sudan I and its' restructured signal only using the approximation coefficient a_j (j=10, 11, 12 and 13). As shown in Fig. 1 (A) and (B), both a_{10} and a_{11} contained all of the components of fluorescence.

From shadows in Fig. 1 (C) and (D), it could be seen that a_{12} and a_{13} did not contained all of the fluorescence components. Therefore, it was better that Raman spectrum of Sudan I was decomposed at level 11.

B. Fluorescence background removal using global thresholding method

Global thresholding method was applied to remove fluorescent background of Sudan I, and three global threshold values of a_{11} were 70000, 80000, 90000 and 100000 . De-nosied and experimental Raman spectrum were shown in Fig. 2.

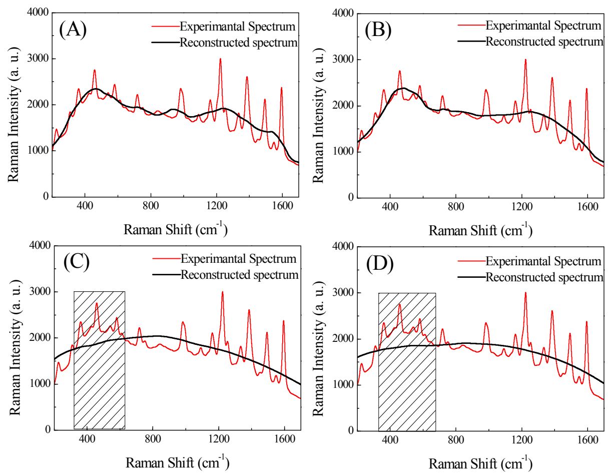

Figure 1. Experimental Raman spectrum of Sudan I and its' restructured signal using the approximation coefficient a_j . (A)-(D) were j=10, 11, 12 and 13 respectively.

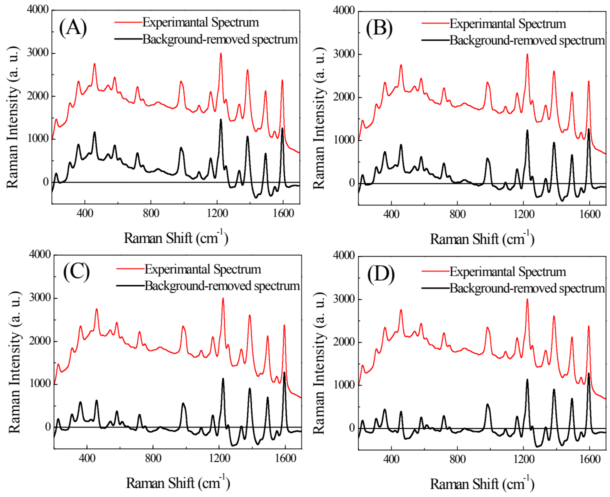

Figure 2. Experimental Raman spectrum and background-removed Raman spectrum using global thresholding method. threshold values of de-noised spectrum shown in (A)-(D) were 70000, 80000, 90000 and 100000 respectively.

From Fig. 2, it was clear that global thresholding method can not remove all the fluorescence background, and restore Raman signal. The reason was that the energy of fluorescence was not homogeneous.

C. Fluorescence background removal using interval thresholding method

Raman spectrum of Sudan I was divided into five parts: (A)-(E), and threshold values of a_{11} in parts (A)-(E) were 9600, 9200, 7800, 6000 and 6400 . The background-removed spectrum was shown in Fig. 3.

As shown in Fig. 3, it could be seen that interval thresholding method can remove all the fluorescence background.

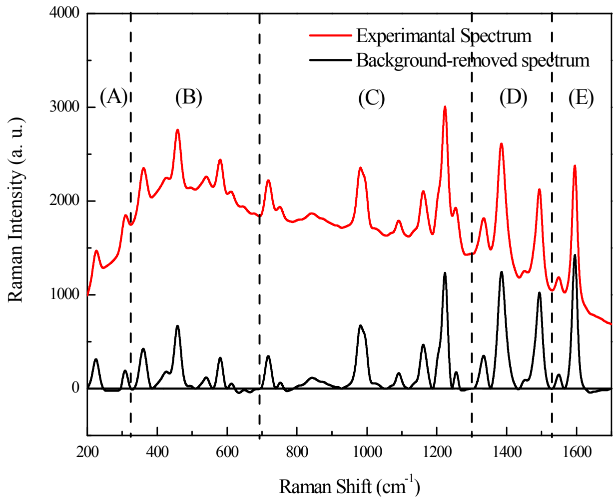

Figure 3. Experimental Raman spectrum and background-removed Raman spectrum using interval thresholding method.

V. CONCLUSIONS

The results indicated that WT is very efficient in removing fluorescence background of Raman spectrum, and the interval thresholding method is more efficient than the global thresholding method.

ACKNOWLEDGMENTS

This research was performed in the photoelectron and information engineering laboratory of Central China Normal University. The authors would like to thank very much all the staffs of the laboratory for their assistance.

REFERENCES

[1] D. A. Tenne, A. Bruchhausen, N. D. Lanzillotti-Kimura, et al, "Probing Nanoscale Ferroelectricity by Ultraviolet Raman Spectroscopy," Science, Vol. 15, Sep. 2006, pp. 1614-1616, doi: 10.1126/science.1130306.

[2] Changhu Yang, Xiaoying Zeng and Jiaxin Liao, "study on Raman spectrum in comparing impurity concentration in water," Environmental Monitoring in China, vol. 24, Feb. 2008, pp. 21-23, doi: CNKI:SUN:IAOB.0.2008-01-006

[3] O. Rioul and M. Vetterli, "Wavelets and Signal Processing," IEEE Signal Processing Magazine, Vol. 8, Oct. 1991, pp. 14-38, doi: 10.1109/79.91217.

[4] S. G. Mallat, "A Theory for Multiresolution Signal Decomposition: The Wavelet Representation," IEEE Transactions on Pattern Analysis and Machine Intelligence, Vol. 11, Jul. 1989, pp. 674-693, doi: 10.1109/34.192463.

[5] C. R. Mittermayr, S. G. Nikolov, H. Hunter and M. Grasserbauer, "Wavelet Denoising of Gaussian Peaks: a Comparative Study," Chemometrics and Intelligent Laboratory Systems, Vol. 34, Sep. 1996, pp.187-202, doi: 10.1016/0169-7439(96)00026-3.

[6] M. P. Wachowiak, G. S. Rash, P. M. Quesada and A. H. Desoky, "Wavelet-based Noise Removal for Biomechanical Signals: A Comparative Study," IEEE T. Bio-Med. Eng. Vol. 47, Mar. 2000, pp.360-368, doi: 10.1109/10.827298.

[7] F. Ehrentreich and L. Sümmchen, "Spike Removal and Denoising of Raman Spectra by Wavelet Transform Methods," Analytical Chemistry, Vol. 73, Jul. 2001, pp.4364-4373, doi: 10.1021/ac0013756.

[8] W. Cai, L. Wang, Z. Pan, J. Zuo, C. Xu and X. Shao, "Application of the Wavelet Transform Method in Quantitative Analysis of Raman Spectra," Journal of Raman Spectroscopy, Vol. 32, Mar. 2001, pp. 207-209, doi: 10.1002/jrs.688 .

[9] P. Hall, G. Kerkyacharian and D. Picard, "Block Threshold Rules for Curve Estmation using Kernel and Wavelet Methods," Ann. Stat., Vol. 26, Jun. 1998, pp.922-942.

[10] P. M. Ramos and I. Ruisánchez, "Noise and Background Removal in Raman Spectra of Ancient Pigments using Wavelet Transform," Journal of Raman Spectroscopy, Vol. 36. Jun. 2005, pp.848-856, doi: 10.1002/jrs.1370.