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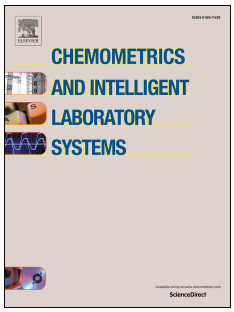

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Minghui Liu, Zuoren Dong, Guofeng Xin, Yanguang Sun, Ronghui Qu

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An improved method based on a new wavelet transform for overlapped peak detection on spectrum obtained by portable Raman system

Liu Minghui,[a,b] Dong Zuoren,[a*] Xin Guofeng,[a] Sun Yanguang,[a] and Qu Ronghui[a]

[a] Key Laboratory of Space Laser Communication and Detection Technology, Shanghai Institute of Optics and Fine Mechanics, Chinese Academy of Sciences, Shanghai 201800, China.

[b] University of Chinese Academy of Science, Beijing 100049, China

Abstract: Peak detection is a particularly important pre-processing step in chemical identification using Raman spectra. At present, most peak detection methods have limited applicability when there are overlapping peaks, especially the spectrum measured by portable spectrometers with low resolution. In this paper, an improved method is proposed based on the application of continuous wavelet transform(CWT) peak detection using a new wavelet to the deconvolved Raman spectrum. The new wavelet has a smaller linewidth and is more similar to the intrinsic Lorentz line profile of the Raman spectrum. It, therefore, has several advantages with regard to the detection of overlapping peaks. The proposed method was evaluated using the Raman spectrum of solid amino acid mixtures, and the results show that it is better at detecting overlapping peaks than the two other investigated wavelets. The receiver operating characteristic curves show that this method can detect more true peaks while maintaining a low false discovery rate. Moreover, the maximum of the true positive rate is the largest in the new approach, which indicates better performance for overlapping peak detection.

Keywords: Raman spectrum; Overlapped peaks; Lorentz4 wavelet; Continuous wavelet transform

1. Introduction

Raman spectroscopy results from the illumination of the substance of interest with a single wavelength laser. The resulting spectrum provides information on molecular bond structure of substance. Therefore, the measured Raman spectrum of a chemical may be used as a “fingerprint” for the purpose of identification. Compared to other analytical techniques, the unique advantages of Raman spectroscopy includes non-destructive and non-contact characterization. In addition, there are no special sample preparation requirements. Moreover, advances in the technical improvement and miniaturization of Raman spectrometric instrumentation have promoted the use of portable instruments for chemical identification in areas such as forensics[1-3], explosives detection[4-6], and geology[7-9], etc. In chemical identification, peak detection is a particularly significant pre-processing step in the analysis of Raman spectra. The accuracy of peak detection directly influences all subsequent analysis. However, due to their low spectrum resolution, the ability of portable Raman spectrometers to identify chemicals is restricted if the chemicals are mixed with others, and the spectrum contains overlapped Raman spectral features. This makes the design of an automatic and accurate peak detection algorithm an urgently necessary but complicated task.

Low resolution of overlapped peaks is a challenging problem for Raman spectrum analysis. In addressing the issue of overlapped peaks, the derivative method[10, 11], Fourier deconvolution method[12-15], wavelet transform method[16-19], and several others are generally applied. In recent years, wavelet analysis has proven to be very successful in a number of signal pre-processing applications such as resolution improvement of composite spectra[20] and feature extraction[21-23]. The continuous wavelet transform (CWT)-based peak detection algorithm has been extensively researched due to its accurate performance and multi-scale property. When the spectrum is transformed into the wavelet space, the algorithm can take advantage of the additional information encoded in the shape of the peaks to reduce the false positive rate. Traditionally, the existing wavelet transform methods for Raman spectrum analysis include the Mexican hat wavelet[16-18] and the Gaus4 wavelet[19]. Du et al. applied CWT for peak detection and directly applied the algorithm to the original spectrum to eliminate the influence of baseline removal[16]. Zhang et al. were able to detect each peak in a spectrum including the ridge, valley and zero-crossing information using multi-scale Mexican hat wavelet space[17]. Zheng et al. presented an improved algorithm that combined the continuous wavelet transform with the crazy climber algorithm. This approach exhibited better performance at identifying overlapped peaks than pre-existing methods[18]. Li et al. proposed a method that combined CWT and curve fitting to obtain the initial parameters of the components in overlapped peaks[19]. The approach is a signal sharpening method for overlapping peaks with noise immunity. Nevertheless, due to the low resolution of portable spectrometers, resolution enhancement is also an urgent problem to be resolved in signal processing of overlapping

* Corresponding author.
E-mail address: zrdong@siom.ac.cn.