De-noising of Raman spectrum signal based on stationary wavelet transform

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In this paper, the Raman spectrum signal de-noising based on stationary wavelet transform is discussed. Haar wavelet is selected to decompose the Raman spectrum signal for several levels based on stationary wavelet transform. The noise mean square σ_j is estimated by the wavelet details at every level, and the wavelet details toward 0 by a threshold $\sigma_j\sqrt{2\ln n}$, where n is length of the detail, then recovery signal is reconstructed. Experimental results show this method not only suppresses noise effectively, but also preserves as many target characteristics of original signal as possible. This de-noising method offers a very attractive alternative to Raman spectrum signal noise suppress.

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Raman spectroscopy is increasingly becoming the preferred tool for material characterization and analysis. It does not only provide a chemical fingerprint of the surface molecules, but also supply additional information concerning the measurement of stress, orientation, midrange order in solids and the identification of surface composition. A major problem with application of Raman spectroscopy is that Raman spectroscopy signal is weak and often overlapped by noise.

Recently, the wavelet transform has received considerable attention from researchers in many areas such as signal processing, image processing, pattern recognition, communication, etc.. The primary attractive feature of wavelet transform is its capacity for multiresolution analysis[1,2]. An important application of wavelets is denoising. A powerful approach for noise reduction based on wavelet transform has been proposed by Donoho and Johnstone[3,4]. It employs thresholding in wavelet domain and has been shown to be asymptotically near optimal for a wide class of signals corrupted by additive white Gaussian noise. It has been successfully applied to the applications such as ECG signal[5] and synthetic aperture radar imaging process[6].

To wavelet multiresolution analysis, Mallat gave the fast discrete wavelet pyramid algorithm[1]. If f_k is discrete sample signal, let $c_{j,k} = f_k$ (in practice, let $c_{0,k} = f_k$ be the initial signal sequence), the Mallat algorithm of signal multiresolution analysis is

$$\begin{cases} c_{j+1,m} = \sum\limits_k \bar{h}(k-2m)c_{j,k} \\ d_{j+1,m} = \sum\limits_k \bar{g}(k-2m)c_{j,k} \end{cases}, \qquad (1)$$

where $c_{j,k}$ represents approximation coefficient of signal, $d_{j,k}$ is detail coefficient of signal. Equation (1) can also be written as

$$\begin{cases} c_{j+1} = D_\varepsilon H c_j \\ d_{j+1} = D_\varepsilon G c_j \end{cases}. \qquad (2)$$

The corresponding reconstruction algorithm is

$$c_{j,k} = \sum_m h(k-2m)c_{j+1,m} + \sum_m g(k-2m)d_{j+1,m}, \quad (3)$$

that is

$$c_j = R_\varepsilon(c_{j+1}, d_{j+1}) = Z_\varepsilon H^* c_{j+1} + Z_\varepsilon G^* d_{j+1}, \qquad (4)$$

where H^* and G^* are conjugate filters of H and G, respectively. D_ε denotes the dyadic downsampling operator, if $\varepsilon = 0$, the operator D_0 simply chooses every even member of a sequence, and if $\varepsilon = 1$, the operator D_1 simply chooses every odd member of a sequence; Z_ε is the dyadic upsampling operator, if $\varepsilon = 0$, the operator Z_0 inserts zeros at odd-indexed elements, and if $\varepsilon = 1$, the operator Z_1 inserts zeros at even-indexed elements; R_ε is reconstruction operator. This is called ε-decimated discrete wavelet transform (DWT).

Suppose the signal is given as[3,4]

$$y_i = f(t_i) + e_i, \qquad (i = 1, 2, \cdots, n) \qquad (5)$$

where $t_i = i/n$, e_i independently distributes as $N(0, \sigma^2)$, and $f(\cdot)$ is an unknown signal which we would like to recover. We measure performance of an estimate $\hat{f}(\cdot)$ in terms of quadratic loss at the sample points. In detail, let $f = (f(t_i))_{i=1}^n$ and $\hat{f} = (\hat{f}(t_i))_{i=1}^n$ denote the vectors of true and estimated sample values, respectively. The performance is measured by the risk of

$$R(\hat{f}, f) = n^{-1} E \left\| \hat{f} - f \right\|_{2,n}^2, \qquad (6)$$

which we would like to make it as small as possible. The procedure of de-noising can be described as follows.

As to noisy signal y_i, let $c_{0,k} = y_i$ denote initial signal sequence, $c_{0,k}$ is decomposed for several times according to Eq. (2), approximation coefficient $c_{j,k}$ and detail coefficients $d_{1,k}$, $d_{2,k}$, $\cdots$, $d_{j,k}$ are obtained. Approximation coefficient $c_{j,k}$ is the main component of true signal, and detail coefficient $d_{j,k}$ contains main component of noise and a few component of true signal wavelet transforms around singular points.

Assume $d_{j,k} = \theta_{j,k} + z_{j,k}$, where $\theta_{j,k}$ is the component of true signal wavelet transform and $z_{j,k}$ is the component of noise wavelet transform. Let $\hat{d}_{j,k}$ be the estimated value of $d_{j,k}$,

$$\hat{d}_{j,k} = \begin{cases} \bar{d}_{j,k} & 1 \le j \le j_0 \\ d_{j,k} & j_0 < j \le J+1 \end{cases}, \qquad (7)$$

where j_0 is low resolution truncation parameter, $\bar{d}_{j,k}$ can be obtained by thresholding detail $d_{j,k}$, threshold is selected as $\sigma\sqrt{2\ln n}$, σ and n are the mean square and length of white noise, respectively. As to white noise, its power is mainly concentrated in first level detail coefficient, and the noise level decreases with the increase of j, so the mean square white noise can be estimated with the first level coefficient, $\sigma = \text{median}(|d_{1,k}|)/0.6745$. Hard thresholding or soft thresholding could be selected to process $d_{j,k}$. Hard thresholding is

$$\bar{d}_{j,k} = \begin{cases} d_{j,k} & |d_{j,k}| \geq \sigma\sqrt{2\ln n} \\ 0 & \text{else} \end{cases}; \quad (8)$$

soft thresholding is

$$\bar{d}_{j,k} = \begin{cases} \text{sgn}(d_{j,k})(|d_{j,k}| - \sigma\sqrt{2\ln n}) & |d_{j,k}| \geq \sigma\sqrt{2\ln n} \\ 0 & \text{else} \end{cases}. \quad (9)$$

The estimated signal $\hat{f}$ is reconstructed from approximation coefficient $c_{j,k}$ and thresholded detail coefficients $\hat{d}_{j,k}$ according to Eq. (4). This de-noising method with the traditional orthogonal wavelet transform sometimes exhibits visual artifacts, and Gibbs phenomena in the neighborhood of discontinuities exhibit after de-noising process.

The undecimated DWT has been independently discovered several times, for different purposes and under different names[7], e.g. shift/translation invariant wavelet transform, stationary wavelet transform, or redundant wavelet transform. The key point is that it is redundant, and it gives a denser approximation provided by the orthogonal DWT.

Suppose the coefficients of the orthogonal wavelet filters H, G are h_j and g_j, respectively, and let Z be the operator that alternates a given sequence with zeros, thus, for all integers j, $(Zx)_{2j} = x_j$ and $(Zx)_{2j+1} = 0$. Define filters $H^{[r]}$ and $G^{[r]}$ to have weights $Z^r h$ and $Z^r g$, respectively, thus the filter $H^{[r]}$ has weights $h^{[r]}_{2^r j} = h_j$ and $h^{[r]}_k = 0$ if k is not a multiple of 2^r. The filter $H^{[r]}$ is obtained by inserting zeros between every adjacent pair of elements of the filter $H^{[r-1]}$, and similarly for $G^{[r]}$. This can be visualized as shown in Fig. 1.

If f_k is an initial discrete signal sequence, let $a_0 = f_k$, $H^{[0]} = H$, $G^{[0]} = G$, signal stationary wavelet transform is

$$\begin{cases} a_{j+1} = H^{[j]} a_j \\ b_{j+1} = G^{[j]} a_j \end{cases}, \quad (10)$$

where a_{j+1} is the approximation coefficient of stationary wavelet transform and b_{j+1} is the detail. Let $a_j(\varepsilon_1, \cdots, \varepsilon_j)$ or $b_j(\varepsilon_1, \cdots, \varepsilon_j)$ denote an approximation or a detail coefficient at level j obtained for ε-decimated DWT and characterized by $\varepsilon = [\varepsilon_1, \cdots, \varepsilon_j]$.

If $\varepsilon_{j+1} = 0$,

$$R^{[j]}_0(a_{j+1}, b_{j+1}) = H^* a_{j+1}(\varepsilon_1, \cdots, \varepsilon_j, \varepsilon_{j+1}) + G^* b_{j+1}(\varepsilon_1, \cdots, \varepsilon_j, \varepsilon_{j+1}), \quad (11)$$

if $\varepsilon_{j+1} = 1$,

$$R^{[j]}_1(a_{j+1}, b_{j+1}) = H^* a_{j+1}(\varepsilon_1, \cdots, \varepsilon_j, \varepsilon_{j+1}) + G^* b_{j+1}(\varepsilon_1, \cdots, \varepsilon_j, \varepsilon_{j+1}). \quad (12)$$

The inverse stationary wavelet transform is

$$a_j(\varepsilon_1, \cdots, \varepsilon_j) = \frac{1}{2}[R^{[j]}_0(a_{j+1}, b_{j+1}) + R^{[j]}_1(a_{j+1}, b_{j+1})]. \quad (13)$$

In Raman spectrum signal de-noising process, we employ thresholding in stationary wavelet transform domain instead of orthogonal wavelet transform domain. This

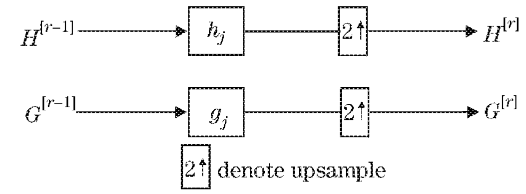

Fig. 1. Filter coefficients upsample processing.

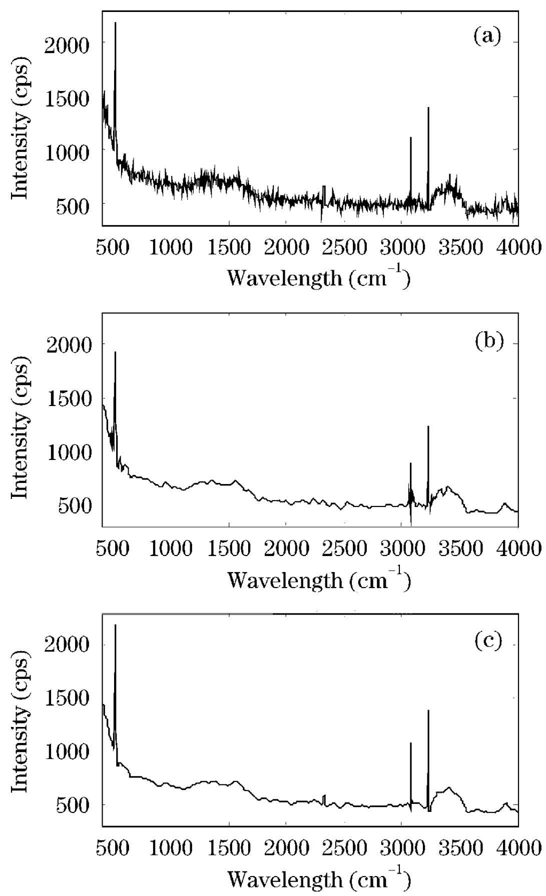

Fig. 2. Experimental results. (a) The Raman spectrum signal of an Ag-MgF_2 nanoparticle cermet film with amorphous MgF_2 matrix and embedded fcc-Ag nanoparticles; (b) the de-noising result by using the de-noising method in Ref. [3]; (c) the de-noising result by stationary wavelet transform.

method can suppress the Gibbs phenomena in de-noising process.

Figure 2(a) is the Raman spectrum signal of an Ag-MgF_2 nanoparticle cermet film with amorphous MgF_2 matrix and embedded fcc-Ag nanoparticles[8]. Figure 2(b) shows the result by using the de-noising method in Ref. [3]. The result shows that in de-noising with orthogonal wavelet transform, the peak around 2320 cm^{-1} vanishes, and Gibbs oscillation appeares around the peak bottoms, such as the positions around 535 and 3080 cm^{-1}, especially the peak bottom around 3080 cm^{-1} is distorted seriously. It is found that Haar wavelet is the best choice in our noise removing experiment with stationary wavelet transform. Figure 2(c) shows the result by stationary Haar wavelet transform. Compared with Fig. 2(b), the peak around 2320 cm^{-1} in Fig. 2(c) appeares clearly and Gibbs oscillations such as that around position 3080 cm^{-1} vanishes.

The proposed technique performs noise removal from the Raman spectrum signal by using normalization of stationary wavelet transform coefficients to make it independent to background intensity, as well as the simple and programmable shrinkage of coefficient by a fixed threshold. The method of noise reduction is fully adaptive, in the sense that it is adaptive to local features by thresholding and to the noise level which varies with both reflectivity level and scale.

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