IJCTA, 9(21), 2016, pp. 297-305

Savitzky–Golay and Wavelet Transform Based Rama Spectroscopic data Denoising

Nitendra Kumar* Khursheed Alam & Abul Hasan Siddiqi*

Abstract **:** Denoising of data or signals has pre-dominantly occupied a considerable position in the present era. Denoising is an important factor that plays an important role in enhancing the quality of the signal. In this paper, denoising of Raman Spectral data of Sr^{+2} 'modified PZT-PMN ceramics (with Sr = 0.0) is done on the basis of Signal to Noise Ratio (SNR). In order to enhance the Raman signal, we have denoised the data to obtain higher SNR. Savitzky-Golay filter and wavelet transform are used for denoising Raman Signals. Savitzky-Golay filter (level 5) and Meyer wavelet (level 3) are being considered for carrying out this work. We have also done a comparative study between Savitzky-Golay filter and wavelet transform.

Keywords : Raman Spectroscopy, Savitzky – Golay Filtering, Wavelet transform

1. INTRODUCTION

Raman spectroscopy is a spectroscopic technique that is based on inelastic scattering of monochromatic light [1]. It is a laser based technique that exploits for qualitative and quantitative biological materials characterization [2]. Raman Phenomenon was discovered by C.V. Raman in the year 1928. Raman devices are more popular and are widely used to improve the security at public places as it is easily portable [3]. The weak nature of Raman Effect results in spectra with very low signal-to-noise ratio (SNR). Raman spectroscopy, a powerful analytical tool that is being used for detection and identification of materials and exhibits high sensitivity to minute biological chemical changes and also helps in providing rich information about the samples [4]. Raman spectroscopy measurements are often affected by the introduction of spurious signals and noise. These noises are mainly produced by thermal noise, shot noise and cosmic rays [1]. In case of biological samples, Raman signal is obscured by a background signal which is due to the intrinsic fluorescence of the organic molecules [4]. Preprocessing of Raman spectroscopy involves spike removal, smoothing or denoising, normalization etc.

1.1. Literature Survey

The first remarkable work was done by Gotman in the year 1982 in the field related to seizures. In 2007, Luis A. Quintero et al worked on denoising of Raman Spectroscopy Signals. They together proposed for an algorithm for removing the impulsive (caused by cosmic rays) that uses a median filter and a classic pattern recognition technique. Also for the second stage for denoising spectra, wavelet is considered and it is compared with the classical smoothening method Savitzky Golay. The algorithms implemented in the work were tested with the synthetic and real spectra. In the work, the performance of the estimation is measured by the mean squared error (MSE) [1]. In the year 2014, Shuo Chen et al worked on recovering Raman Spectra with low signal to noise ratio using Weiner estimation. Their work includes synthesis of narrow-band measurements from low-SNR Raman spectra which eliminates the effect of noise by integrating the Raman signal along the wavenumber dimension. Later it is followed by the spectral reconstruction that is based on Wiener estimation for the recovery of Raman spectrum with high spectral resolution. To ensure that the most variance contained in the original Raman measurements are

* School of Engineering & Technology, Department of Applied Science, P.N.: 32-34, Knowledge Park -3, Sharda University, Greater Noida 201306 Email: nkshukla.kumar4@gmail.com, khursheed.alam@sharda.ac.in, siddiqi.abulhasan@gmail.com

retained, they introduced Non-negative principal components based filters for synthesis purpose. A total of 25 agar phantoms and 20 bacteria samples were measured. And these data were used to validate the method. De-noising methods such as Savitzky-Golay (SG) algorithm, finite impulse response (FIR) filtration, wavelet transform and factor analysis were also evaluated on the same set of data in addition to the proposed method for comparison. Superior accuracy in the recovery of Raman spectra from measurements with extremely low SNR, in comparison with the four commonly used de-noising methods were shown in the proposed work [2]. F. Ehrentreich et al proposed denoising and spike removal of Raman spectra by using wavelet transform (WT) methods. In their work the wavelet transform was applied in repetitive mode for sequential analysis: preliminary denoising, despiking and also refined denoising. C. M. Galloway et al introduced an algorithm based on wavelet transforms for background removal in Raman spectroscopy.

1.2. Types of Noise

Mainly noise in Raman spectra takes one of these forms: low-frequency noise, high frequency noise, and cosmic spikes. High frequency noise is due to the data acquisition electronic circuit and other sources of system variation, low frequency noise arise from ambient light entering the spectrograph and fluorescence that is due to the induction of laser beam [3]. Cosmic spikes are spurious, and appear as very narrow spikes in the Raman spectra. Other important sources of noise are: signal shot noise, dark noise and readout noise [1, 24].

2. METHODOLOGY

It is a well known fact, for a scientist or an engineer working with a real data knows that signals do not exist without noise. The noise corrupts the signal in a significant manner and for further analysis the signal has to be made noise free. Signal denoising which is referred recovery of a signal from noise plays an important role for enhancing signal to noise ratio (SNR). In this work the denoising of Raman signals are based on Savitzky-Golay Smoothing and Wavelet Transform.

2.1. Savitzky – Golay Smoothing Filtering

Savitzky and Golay in 1964 together proposed a method for smoothing data which was based on least-squares polynomial approximation fitting within a window [7] and also based on polynomial regression [9]. Data smoothing is simply a process of improving the visual appearance of a recorded signal trace by the suppression on noise and also making very little effect on the signal. It also provides an alternative to moving point average smoothing. Savitzky-Golay smoothing filters are basically derived from the field of numerical analysis and were first investigated in time domain. Savitzky-Golay smoothing filters helps in reproduction of the polynomials, reduction and amplification of noise and also in preserving small details [8]. Savitzky-Golay is basically a digital filter as it is applied to a set of digital data points for smoothing so to increase the signal to noise ratio (SNR) without much distorting the signal and also the shape and height of waveform are maintained. To improve the smoothing results, Savitzky- Golay filter employs the regression fitting capacity. Due to the advantage of the fitting ability of polynomial regression, it performs better than moving window average. Savitzky-Golay filter is essentially a weighted average method in the form of and it is one of the major differences between Savitzky-Golay filter and moving-window average method [9]. Hence Savitzky-Golay filter smoothes the signal or noise component by using piece by piece fitting of a polynomial function and this fitting is carried by the minimization of least squares measure [3].

$$X_1^* = \frac{1}{2m+1} \sum_{j=-m}^{m} W_j X_{i+j} \quad ...(1)$$

Moving-Window Average Smoothing Method : It is the simplest smoothing method and it is utilized for the enhancement of SNR.

$$X_1^* = \frac{1}{2m+1}\sum_{j=-m}^{m} X_{i+j} \qquad ...(2)$$

Where X_1^* denotes the smoothed value, X_{i+j} as original raw data and *i*, *j* are running indices.

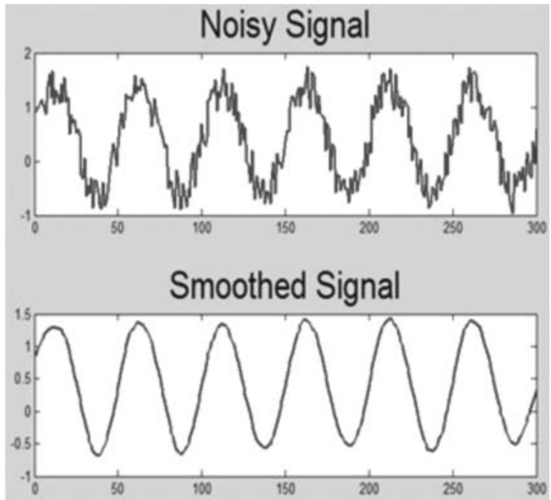

Fig. 1. Plot of Noisy and Smoothed Signal

2.2. Wavelet Transform

The arrival of wavelets started with the failure of Fourier series as it resolved the problems of Fourier Transform (FT), Fast Fourier Transform (FFT) and Short Time Fourier Transform (STFT). Wavelet transform has been an efficient tool for signal analysis as it holds the property of multiresolution [11]. Wavelets are much more concentrated in time in comparison to other techniques such as Fourier Transform.

Continuous Wavelet Transform (CWT) : Mathematically, Continuous wavelet transform (CWT) with respect to some local base function is defined by [12]

$$W(a, b) = W_W f(b, a) = \frac{1}{\sqrt{a}}\int_{-\infty}^{+\infty} f(t)\, \psi^*\left(\frac{t-b}{a}\right) dt,\ a > 0 \qquad ...(3)$$

here '*b*' and '*a*' are translation and dilation parameter. *f*(*t*) represents the analyzed signal.

Properties of CWT :

$$\int_{-\infty}^{\infty} \psi(t)\, dt = 0 \qquad ...(4)$$

$$\int_{-\infty}^{\infty} |\psi(t)|^2 dt < \infty = 0 \qquad ...(5)$$

here $\psi(t)$is called as mother wavelet or simply a basic wavelet.

CWT also has one admissibility condition, given by :

$$C = \int_{-\infty}^{\infty} \frac{|\Psi(\omega)|^2}{|\omega|} d\omega; 0 < C < \infty \qquad ...(6)$$

Discrete Wavelet Transform (DWT) : Discrete wavelet transform (DWT), helps in transforming a discrete time signal into a discrete wavelet representation. The discrete wavelet series is simply a sampled version of the continuous wavelet transform and the information provided by it is highly redundant as far as the reconstruction of the signal is concerned. DWT is easy to implement in comparison to CWT. Discrete wavelets are applied to discrete data sets and produce discrete outputs. The main difference between the discrete and continuous wavelet transform is the choice of the possible values for the (a, b) variables. In CWT we can't put any constraints on the choice of these two coordinates and they can in principle map the whole (a, b) plane [13]. In the discrete wavelet transform, however, we restrict the choice of possible (a, b) values as follows:

$$a = a_0^j, b = kb_0 a_0^j$$

DWT decomposes the signal into mutually orthogonal set of wavelets and this is the main difference of DWT from CWT.

$$\psi_{j,k}(t) = \frac{1}{\sqrt{s_0^j}} \Psi\left(\frac{t - k\tau_0 s_0^j}{s_0^j}\right)$$

Where j and k are integers and $s0 > 1$ is a fixed dilation step. The translation factor t_0 depends on the dilation step.

Wavelet Denoising : Wavelet denoising is based on some criteria for the selection of optimal wavelets. Denoising helps in removing noisy components by proper selection of thresholding. Wavelets with more vanishing moments, better reconstruction and less distortion properties are selected. Also while denoising the important information can be retained [14].

Wavelet Thresholding : Thresholding is a signal estimation technique used for exploiting the capabilities of signal denoising. Normally thresholding categorizes itself into two types: hard thresholding and soft thresholding [14].

Hard Thresholding : It is the simplest type of thresholding but somehow it lacks nice mathematical properties. Here 'T' is the threshold.

$$y = \begin{Bmatrix} x, |x| > \mathrm{T} \\ 0, |x| < \mathrm{T} \end{Bmatrix} \qquad \text{...(9)}$$

Soft Thresholding : It is an extension to hard thresholding and has better mathematical properties in comparison to hard thresholding. Here 'T' is the threshold.

$$y = \begin{Bmatrix} \mathrm{sign}(x).(|x| - \mathrm{T}), |x| > \mathrm{T} \\ 0, |x| < \mathrm{T} \end{Bmatrix} \qquad \text{...(10)}$$

Thresholding Rules : Denoising of signals based on fixed thresholding was initially proposed by D. L. Donoho and the value of threshold is given by

$$t = \sigma\sqrt{2\log(n)/n} \qquad \text{...(11)}$$

Where $\sigma = \frac{\mathrm{MAD}}{0.6745}$, MAD is the median of the wavelet coefficients and 'n' is the total number of wavelet coefficients [11].

Denoising Algorithm : $y(n) = x(n) + w(n)$ ...(12)

Where $x(n)$ – signal to be detected

$y(n)$ – resultant signal or required signal and

$w(n)$ – noise (generally white Gaussian noise).

3. DATA TYPE

Raman Spectral data of Sr^{+2}'modified PZT–PMN ceramics (with Sr = 0.0) has been collected by Raman spectrometer of Remisaw Rm–1000 spectroscope, which use 1.19 nm as a unit the range of 200–1000 cm^{-1}. The experiment was carried at a room temperature about 25°C. The data has been obtain in .txt format and has two kinds of 876X2 data that represents the intensity–Raman shift and the intensity–pixel. Export the intensity value (876X1 only and take it as one-dimensional signal).

4. EXPERIMENTAL RESULTS AND DISCUSSION

In this proposed work, we have denoised Raman Spectral data of Sr^{+2} ‘modified PZT-PMN ceramics (with Sr = 0.0) using Savitzky-Golay smoothing filter and wavelet transform. The denosing work is based on signal to noise ratio (SNR). For wavelet denoising, we have considered Meyer wavelet. The decomposition level selected for Savitzky-Golay filter and wavelet transform is 5 (*i.e*. N = 5). We have carried out this denoising work on MATLAB software. Also we have compared Savitzky-Golay denoising results with the denoising results of wavelet transform.

4.1. Signal to Noise Ration (SNR)

It is defined as the ratio of signal power to noise power of the signal. It gives the strength of the signal and it is usually expressed in decibels (dB) [14].

$$\text{SNR} = \text{Signal Power / Noise Power.}$$

$$\text{SNR}(db) = 10\ln \frac{\sum_{k=1}^{N} x^2(k)}{\sum_{k=1}^{N} [x(k) - x'(k)]^2} \quad \text{...(13)}$$

4.2. Savitzky-Golay Denoising Procedure

The denoising procedure were carried on MATLAB software. The filter level chosen to carry out denoising at level 5 (N = 5). The signal to noise ratio have been carried out 40.1672.

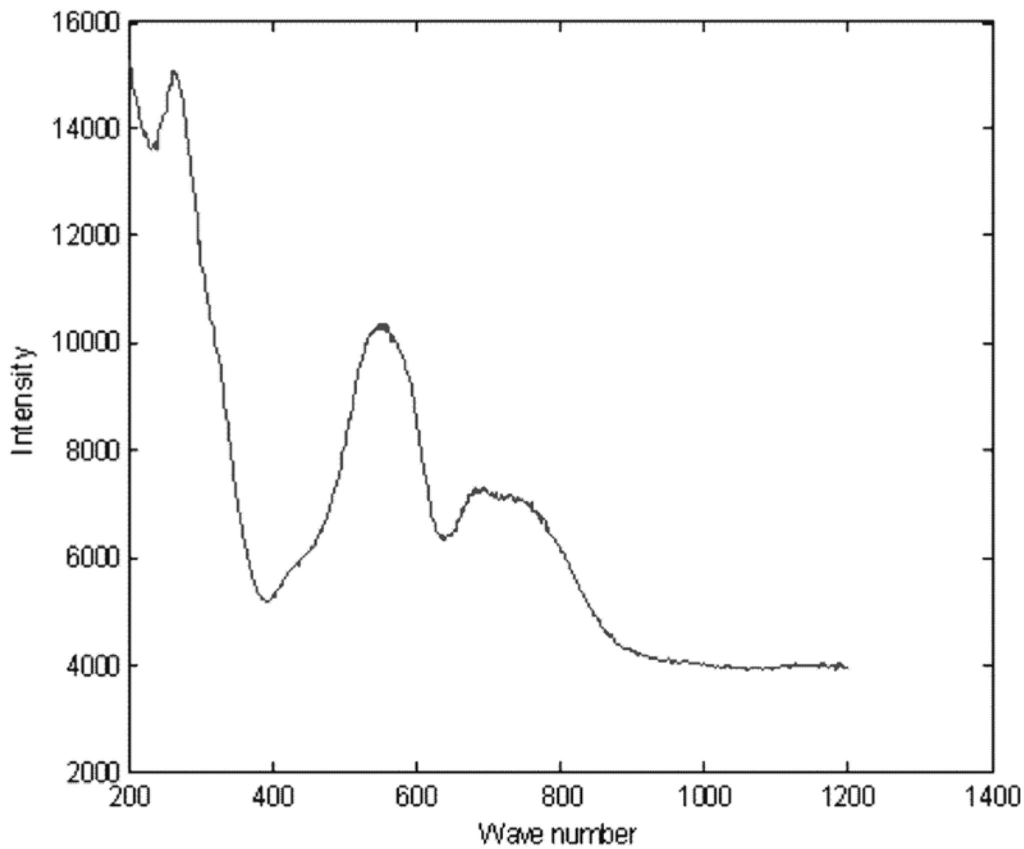

Fig. 2. Plot of Original Raman Spectra

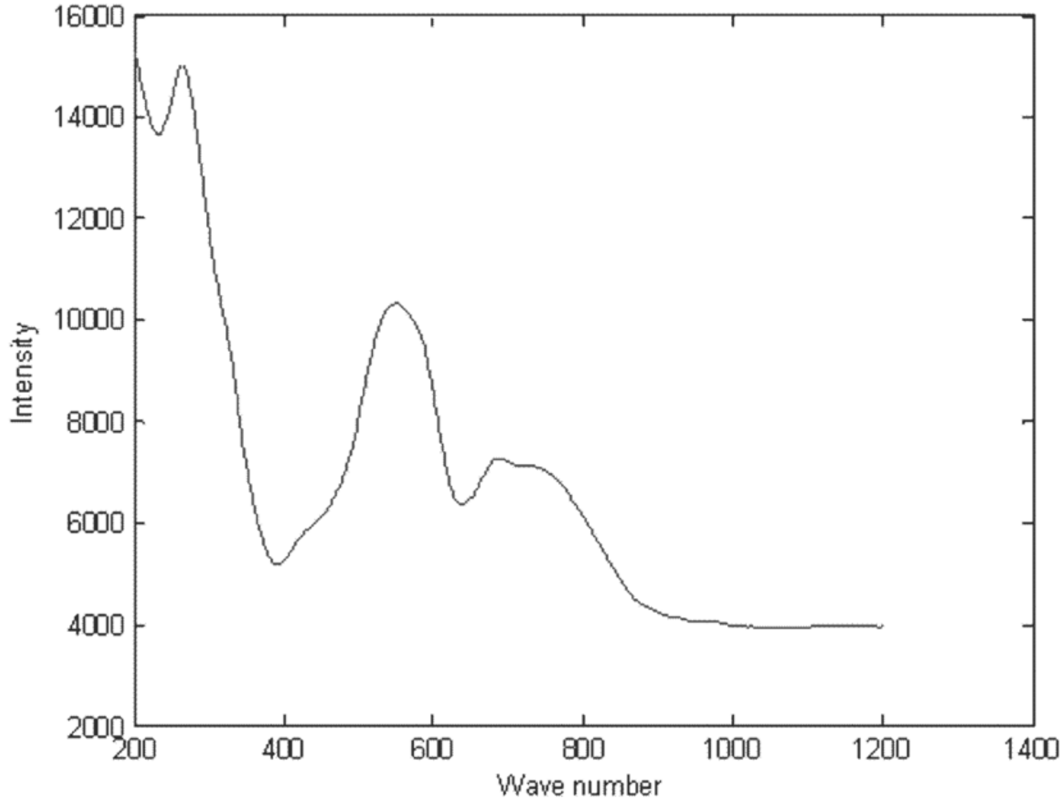

Fig. 3. Denoising of Raman Spectra at Golay (N = 5)

4.3 Meyer Wavelet

Meyer wavelet (dmey) is basically an orthogonal wavelet, with symmetry and scaling functions. It was proposed by Yves Meyer. Meyer wavelet function is a frequency band-limited function whose Fourier transforms has a compact support, namely, nonzero and that is only in a finite interval of frequency variable ω. In Meyer wavelet the resultant scaling function $\phi(x)$ is defined by its Fourier Transform. Also Meyer wavelet function $\psi(x)$ and Meyer scaling function $\phi(x)$ do not have compact support *i.e.* $\psi(x) \neq 0$ and $\phi(x) \neq 0$ for any 'x' except for some points. In Meyer wavelet these functions do decrease to 0 when $x \to \infty$ at a very high speed. These two functions of Meyer wavelet have better regularity and are infinitely differentiable. Meyer wavelet functions have infinite number of vanishing moments [10].

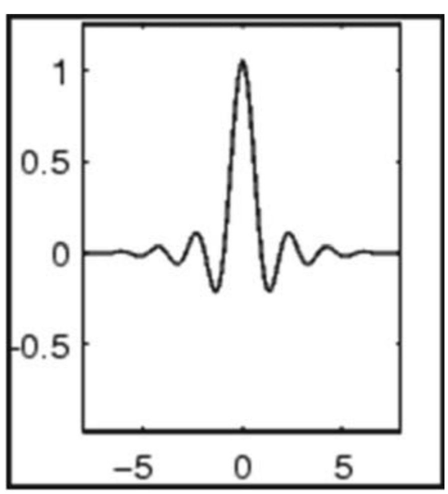

Fig. 4. Meyer Scaling Function

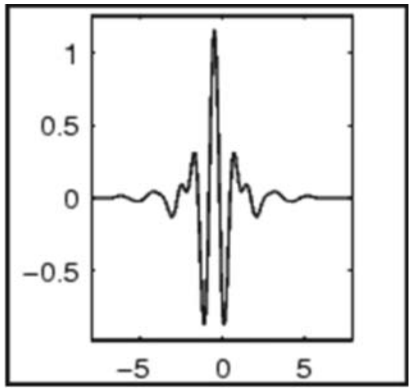

Fig. 5. Meyer Wavelet Function

4.4. Wavelet Denoising Procedure

The decomposition of input signal is done using Discrete Wavelet Transform (DWT). Generally the denoising procedure involves three steps [15]:

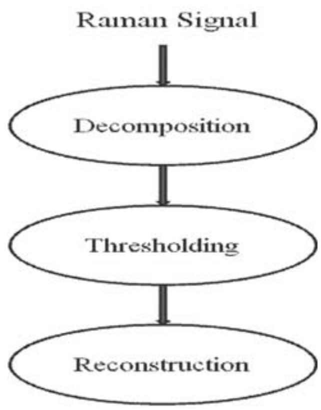

Fig. 6. Signal Decomposition using Wavelet Transform

In decomposition, we choose a wavelet and select a level 'N' i.e. 5, we have selected for Meyer wavelet being used in this work for decomposition. Now we compute the decomposition of Raman signal at level '5'. After decomposition, we select thresholding method. In this we select a threshold for each level of wavelet decomposition i.e. from 1 to 5. For carrying out this work we have selected hard and soft thresholding. The signal to noise for soft and hard thresholding have been calculated as 39.5967 and 41.4768 respectively.

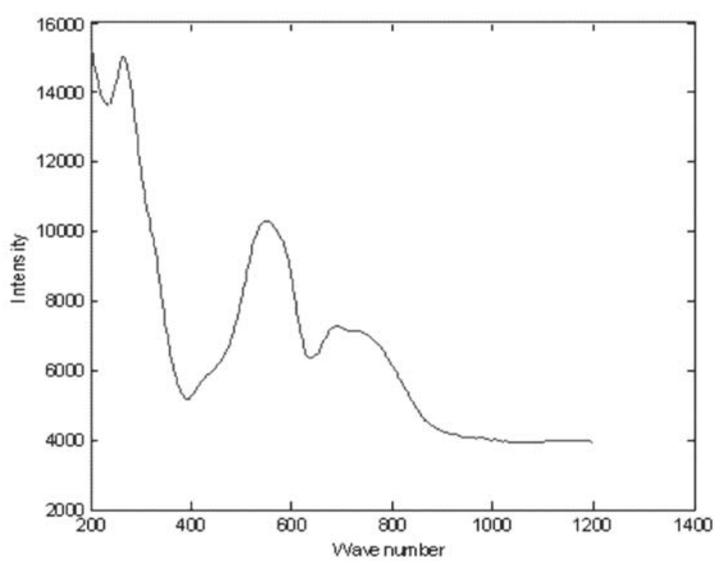

Fig. 7. Denoising Plot at Meyer Wavelet (Level 5, soft thresholding)

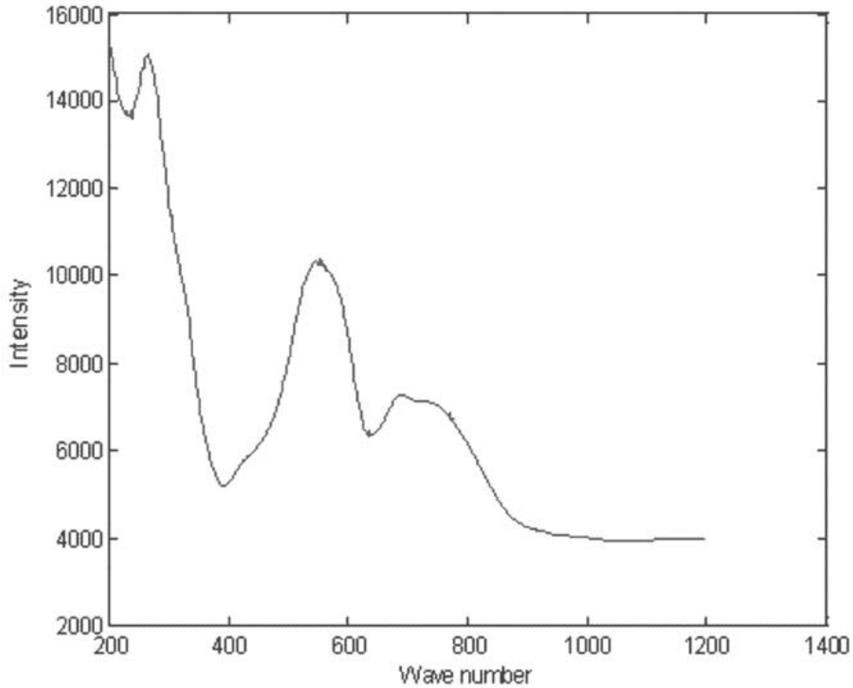

Fig. 8. Denoising Plot at Meyer Wavelet (Level 5, hard thresholding)

5. CONCLUSION

In this article, Savitzky – Golay and Meyer wavelet with decomposition level 5, for Meyer Wavelet choosing soft and hard thresholding with scaling white noise, have been used for denosing of Raman spectra of Sr^{2+} modified PMN-PZT ceramics. Best result performed at Meyer Wavelet at hard thresholding.

6. REFERENCES

1. Luis A. Quitero, Shaun Hunt and Max Diem, "Denoising of Raman Spectroscopy Signals" Bernard M. Gordon Center for Subsurface Sensing and Imaging Systems (Gordon-CenSSIS), January 01, 2007.
2. Andrzej Kwiatkowski, Marcin Gnyba, Janusz Smulko and Pawe³ Wierzba, "Algorithms of Chemical Detection using Raman Spectra", *Polish Academy of Science,* Vol - XVII, No.- 4. pp 549-560, 2010.
3. Nikolaos Kourkoumelis, Alexandros Polymeros and Margaret Tzaphlidou, 'Background Estimation of Biomedical Raman Spectra Using a Geometric Approach", *Hindawi Publishing Corporation Spectroscopy: An International Journal*. Vo l-27. pp 311-317, 2012.
4. F. Ehrentreich and L. Su1mmchen, "Spike Removal and Denoising of Raman Spectra by Wavelet Transform Methods", *American Chemical Society*. Vol - 73, No.-17. pp 4364-4373, 2001.
5. C. M. Galloway, E. C. Le Ru and P.G. Etchegoin, "An Iterative Algorithm for Background Removal in Spectroscopy by Wavelet Transforms" *Applied Spectroscopy*. Vol - 63, No. - 12. pp 1370-1376, 2009.
6. Ronald W. Schafer, "On the Frequency-Domain Properties of Savitzky-Golay Filters". *Hewlett-Packard Development Company, L.P, 2010*.
7. S Hargittai, "Savitzky-Golay Least-Squares Polynomial Filters in ECG Signal Processing" *Computers in Cardiology.* IEEE. pp 763-766, 2005.
8. Foo-Tim, Yi-zeng Liang, Junbin Gao and Xue – Guang Shao, "Chemometrics From Basics to Wavelet Transform", *Wiley – Interscience*. Vol - 164. pp 99-141, 2004.
9. Sai Lakshmi Bhamidipati, Sai Sudha Mindagudla, Harsha Vardhan Devalla, Hima Sagar Goodi and Hemnath Nag, "Analysis of Different Discrete Wavelet Transform Basis Functions in Speech Signal Compression". *IOSR Journal of VLSI and Signal Processing (IOSR-JVSP)*. Vol -4, pp 34-38, 2004.
10. P.Karthikeyan, M. Murugappan and S.Yaacob, "ECG Signal Denoising UsinG Wavelet Thresholding Techniques in Human Stress Assessment", *International Journal of Electrical and Informatics*, Vol - 4, No.-2, pp 306-318, 2012.

11. A. H. Siddiqi, R. C. Singh, P. Manchanda, "Proceedings of Satellite Conference ICM 2010 on Mathematics in Science and Technology", *World Scientific Publisher*, Singapore, 2011.

12. Bjorn K. Alsberg, Andrew M. Woodward and Douglas B. Kell. "An Introduction to Wavelet Transforms for Chemometrics: A time – frequency approach" *Chemometrics and Intelligent Laboratory Systems, Elsevie.r*. Vol – 37. pp 215-239, 1997.

13. Nitendra Kumar, A. H. Siddiqi and Khursheed Alam, "Raman Spectral Data De-noising based on Wavelet Analysis", *International Journal of Computer Applications*, Volume 102– No.16, 2014.

14. Gautam Kumar, Sugandh Kumar and Nitendra Kumar, "Comparative Study of Wavelet and Wavelet Packet Transform for Denoising Telephonic Speech Signal". *International Journal of Computer Application (IJCA)*, Vol – 110. No.-15. pp 1-22, 2015.

15. C. V. Raman & K. S. Krishnan, " A New Type of Secondary Radiation", *Nature*, 121, pp 501-502, 1928.

16. Mahesh S. Chavan and Nikos Mastorakis, "Studies on implementation of Meyer and Daubechies Wavelet for Denoising of Speech Signal" *International Journal of Circuits, Systems and Signal Processing*, Vol -4, Issue 3. pp 83-96, 2010.

17. I. Daubechies, S. Mallat and A.S. Willsky, "Special Issue on Wavelet Transforms and Multiresolution signal Analysis Introduction", *IEEE Trans. Inf. Theory,* Vol – 38. pp 529-531, 1992.

18. D. L. Donoho, "De-noising by Soft-Thresholding", *IEEE Trans. Inf. Theory,* Vol – 41. No. 61. pp 613-627, 1995.

19. F.T. Chau, A.K.M. Leung, J.B. Gao and T. M. Shih, "Application of wavelet Transform in infrared spectrometry", *Spectral compression and library search.*, Vol – 43. pp 69-88, 1998.

20. P. L. Ainsleigh and C. K. Chui, "A B-wavelet-based noise-reduction algorithm. *IEEE Transaction. Signal Processing*, Vol. - 44. pp 1279-1284, 1996.

21. P. M. Ramos and I. Ruis´anchez, "Noise and Background Removal in Raman spectra of Ancient Pigments using Wavelet Transform, *Journal of Raman Spectroscopy*, Vol -36, No. 9. pp 848–856, 2005.

22. I. Daubechies, "Ten Lectures on Wavelets". *SIAM Press.* Philadelphia, ISBN:0-89871-274-2, 1992.

23. Amara Graps, "An Introduction to Wavelets", *IEEE Computation Science and Engineering*. Vol. - 2, Issue 2. pp 50-61, 1995.

24. Rekha Gautam, Sandeep Vanga, Freek Ariese and Siva Umapathy **, "**Review of multidimensional data processing approaches for Raman and infrared spectroscopy**",** *EPJ Techniques and Instrumentation, Springer Open,* DOI: 10.1140/ epjti/s40485-015-0018-6, 2015.