

# Terahertz Time-Domain Spectroscopy Analysis with Wave Atoms Transform

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**Abstract**—In this paper, a terahertz time-domain spectroscopy analysis method is proposed based on wave atoms transform. As reflection happens when the terahertz goes through the surface of the substance, the traditional Fourier Transform analysis or other transforms analysis like wavelet and curvelet has a limitation on providing clear spectrum characteristics of a wave. Compared with conventional methods, wave atoms transform has sparser expansion for the oscillatory and oriented textures, which is expected to have a better performance when dealing with wave reflection phenomenon. The experimental results demonstrate that the proposed method can enlarge the resolution in the frequency domain; a number of covered significant spectrums are refined. According to the results, the proposed method is most suitable for the spectrums which have one or two distinct wave crests. For the spectrums which are steadily decreasing, the improvement is not significant. Overall, compared with the conventional analysis methods, the proposed method achieves a better spectrum performance.

## I. INTRODUCTION

Terahertz radiation is the wave that has the frequency at 0.1THz to 10THz. It locates between microwave and infrared wave region of the electromagnetic spectrum. Due to the rich physical and chemical characteristics in this region, it has a great importance in analyzing the spectrum of the matters in this region. THz time domain spectroscopy is a very promising technique for its unique time-resolved feature and high signal to noise ratio (SNR) at THz frequency [1-5]. The typical THz time domain spectroscopy system is constructed by a femtosecond laser, a THz emitter generator, a THz detector and a time delay system [1, 6]. The principle of THz time domain spectroscopy is described as follows: A laser generated by femtosecond laser will be divided into two beams when passing the beam-splitter. And then one of the beams will go through the time delay system and reach to the THz emitter to generate THz radiation. Another beam will go through the material which is detected together with the THz generated by the first beam. By adjusting the time delay between these two beams, we can obtain the pulse reflected by the material [7-9]. The THz signal of the material is known, by analyzing the spectrum of the signal; the material's THz spectral property can be shown. The conventional THz-TDS analysis is based on Fourier Transform (FT) [10]. The entire THz pulse will be translated into frequency domain by

applying FT. But when the THz wave goes through the detected substance, reflection may happen between substrate boundaries which will result in signal overlapping in the frequency domain. Moreover, the noise caused by laser fluctuation will also be added into the original signal. Therefore, the resolution of the signal in frequency reduced as spectral convolution occurred and some significant spectral characteristics are often covered up. As we know that wave atoms have a sparser expansion for the oscillatory and oriented textures [11], we introduce the wave atom transform into the THz-TDS analysis in order to improve the spectral results. In recent years, wave atoms transform has been applied into signal and image processing such as watermarking, image de-noising and etc. However, there is a lack of a 1D wave atoms investigation in these areas. The purpose of this article is to investigate the effect of applying wave atoms in THz-TDS spectral analysis.

When a wave goes through the interface between two media which have different material densities, reflection happens. In fact, there is only part of the wave being reflected. And when a wave goes through a boundary, part of the waves will be absorbed by the material and some energy of the wave will also be dissipated. In THz-TDS system, the substance has two boundaries. The first refracted wave will transmit to the other interface which will generate the second reflected wave. The second wave will then transmit back to the first interface and then generate a new reflected wave and a new refracted wave, iteratively.

Hence, the final received wave at the first boundary will be the sum of the reflected wave from the front surface and other refracted waves passing through the front surface which is reflected from the back surface. Note that a multiplication of two signals in time domain will result in a convolution in frequency domain. It shows that some refracted waves are masked by high frequency components. Thus the resolution in frequency domain will be decreased. So it is obvious that the traditional Fourier Transform has limitations on providing clear spectrum characteristics of a wave with inherited reflection behavior.

## II. WAVE ATOM TRANSFORM

It was first introduced by Demanet and Ying [12] that wave atoms are variant of 2-D wavelet packets and obey the parabolic scaling law  $wavelength \sim (diameter)^2$ . It can adapt to arbitrary local directions of a pattern, and also can sparsely represent anisotropic patterns aligned with the axes. Oscillatory functions and oriented textures in wave atoms have been proved to have a dramatically sparser expansion compared to some other fixed standard representations like Gabor filters, wavelets, and curvelets. Wave atoms interpolate precisely between Gabor atoms [13] and directional wavelets [14], and the period of oscillations of each wave packet (wavelength) is related to the size of essential support via parabolic scaling i.e.  $wavelength \sim (diameter)^2$  while for wavelet  $diameter \sim wavelength$  and for Gabor  $diameter \sim wavelength^0 = const$ .

#### A. Definition of Wave Atoms

Wave atoms are defined as  $\varphi_\mu(x)$  with subscript  $\mu = (j, \mathbf{m}, \mathbf{n}) = (j, m_1, m_2, n_1, n_2)$ , where  $j, m_1, m_2, n_1, n_2$  are all integer value and index a point  $(x_\mu, \omega_\mu)$  in phase-space, as

$$x_\mu = 2^{-j} \mathbf{n}, \omega_\mu = \pi 2^j \mathbf{m}, C_1 2^j \leq_{i=1,2} |m_i| \leq C_2 2^j \quad (1)$$

where  $C_1$  and  $C_2$  are two positive constants, the position vector  $x_\mu$  is the center of  $\varphi_\mu(x)$ , and  $\omega_\mu$  is the wave vector which determines the center of both bumps  $\hat{\varphi}_\mu(\omega)$  as  $\pm \omega_\mu$ .

#### B. 1D Discrete Wave Atoms Implementation

Wave atoms are constructed from tensor products of 1-D wave packets in practice. Now we define  $\psi_{m,n}^j(x) = \psi_m^j(x - 2^{(-j)}n) = 2^{j/2} \psi_m^0(2^{-j}x - n)$  as a 1D wave packet, where  $j \geq 0, m \geq 0, n \in \mathbb{Z}$ . In space, it is centered around  $x_{j,n} = 2^{-j}n$ . And in frequency it is centered around  $\pm \omega_{j,m} = \pm \pi 2^j m$  with  $C_1 2^j \leq m \leq C_2 2^j$ . The  $\psi_m^0(\omega)$  is defined as

$$\psi_m^0(\omega) = e^{-i\omega/2} [e^{i\alpha_m} g(\epsilon_m(\omega - \pi(m+1/2))) + e^{-i\alpha_m} g(\epsilon_m(\omega - \pi(m+1/2)))] \quad (2)$$

Where  $\alpha_m = \frac{\pi}{2}(m + \frac{1}{2})$ ,  $\epsilon_m = (-1)^m a$  and a real-value  $g$  and compactly-support  $C^\infty$  bump function with  $\sum_m |\psi_m^0(\omega)|^2 = 1$ .

For each wave  $w_{j,m}$  at scale  $2^{-j}$  the coefficient  $c_{j,m,n}$  can be treated as a decimated convolution. By discretizing the sample  $u$  at  $x_k = kh, h = 1/N, k = 1, \dots, N$ , the discrete

coefficients  $c_{j,m,n}^D$  are computed using a reduced inverse FFT inside an interval of size  $2^{j+1}\pi$  centered about the origin.

$$c_{j,m,n}^D = \sum_{k=2\pi\left(-\frac{2^j}{2}+1, \frac{1:2^j}{2}\right)} e^{i 2^{-j}nk} \sum_{p \in 2\pi\mathbb{Z}} \hat{\psi}_m^j(k + 2^j p) \hat{u}(k + 2^j p) \quad (3)$$

### III. TERAHERTZ SPECTRAL ANALYSIS WITH WAVE ATOMS

According to the properties of wave atoms, we consider that it is probably a better match to reflected wave in THz spectrum analysis. Hence, we proposed a new method to analyze the THz pulse using wave atoms. The data we used are from RIKEN Sendai [15], a Japanese THz research institute. The data provided by the RIKEN database are all presented in frequency domain. In order to restore the original wave format, a pre-processing is made on the RIKEN's data by assigning the phase all to zero and then performing the inverse Fourier Transform. When we obtain the time domain wave form, we can apply wave atoms transform to it. After applying the wave atoms transform, the entire signal information will be dispersed to several scale bands. And each band is made up of several matrixes with different sizes. The coefficients in the matrix represent the signal information in wave atom. In our cases, the number of scale bands is made between six and eight. Figure 1 illustrates the details of the proposed method.

1. Apply inverse Fourier Transform to the original spectrum  $I$ , and the signal  $I'$  is obtained in the time domain.
2. Apply wave atoms transform to  $I'$ . Define  $C\{Si\}$  as the entire signal after being applied with wave atoms, where  $S_i$  represents each scale band,  $i = 1, 2, \dots, 8$ . and  $C\{Si\} = S_1 + S_2 + \dots + S_i$ .
3. To investigate the characteristics of each single scale band, it can be analyzed individually by setting the values in matrix of other scale bands to zero except the target band. First, we denote  $Ci\{Si\}$  to represent each scale band, where  $i = 1, 2, \dots, 8$ ,  $j = 1, 2, \dots, 8$ . And  $Cj\{Si\} = S_j + S_1 + \dots + S_{j-1} + S_i$ , where  $|S_1|, \dots, |S_j|, |S_{j+1}|, \dots, |S_i| = 0$ . For example, if we want to obtain the first scale band's wave form, then  $C\{S1\} = S1$ , and we will set the coefficients in the other scale bands to zero, i.e.  $|S_2|, |S_3|, \dots, |S_i| = 0$ .
4. After obtaining every single scale band's data, inverse wave atoms transform is applied to every  $Ci\{Si\}$ , where  $i = 1, 2, \dots, 8$  and  $j = 1, 2, \dots, 8$ . Then we will obtain the time domain signal of every single scale band, recording it as  $T_j$ , where  $j = 1, 2, \dots, 8$ .

- Apply the Fourier transform to every  $T_j$ . Then the spectrum  $T'_j$  of each scale band is obtained in the frequency domain.

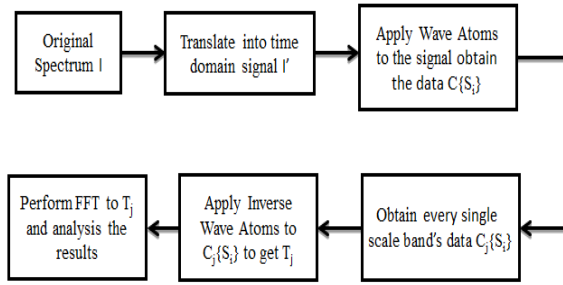
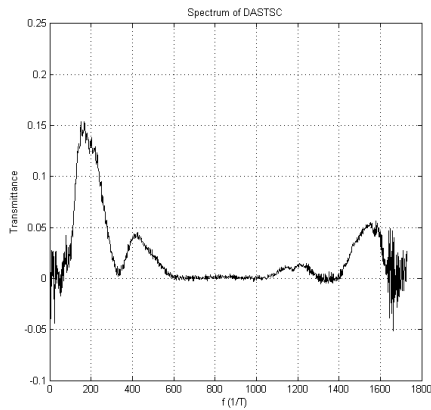


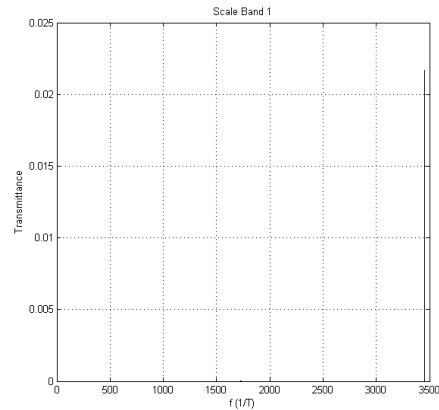
Fig. 1 Flow chart of proposed method

In order to guarantee the validity of the data,  $T_1, T_2 \dots T_j$  are added together to obtain the wave form and then compare with  $I'$  to check whether there is a loss of data. After applying the proposed method, a group of spectrums  $\{T'_j\}$  is obtained. Then we can compare it with the traditional spectrum which is processed by the Fourier Transform. Using the wave atoms transform, the signal is usually represented as a complex number. In order to sketch the wave form and the spectrum, only real part is used. And the number of scale band is variable with the input.

#### IV. EXPERIMENTAL RESULTS



a



b

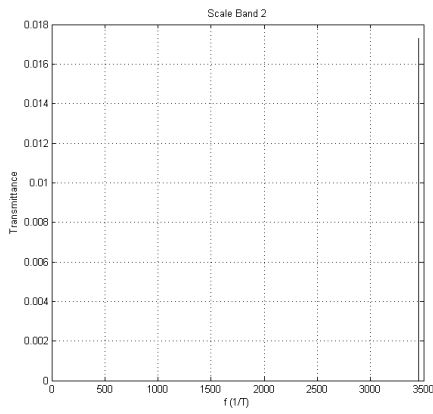
The experimental results of the proposed THz-TDS analysis method are presented in this section. Due to the reflection, there are echo pulses in the time domain. Therefore, interference occurs in the frequency domain. The aim of using the wave atom transform is to improve the frequency resolution. A number of spectrums are tested in total and some significant results are obtained.

Figure 2 shows a typical case of the absorption spectra of 4-dimethylamino-N-methyl-4-stilbazolium tosylate and its 7 scale bands processed after wave atoms.

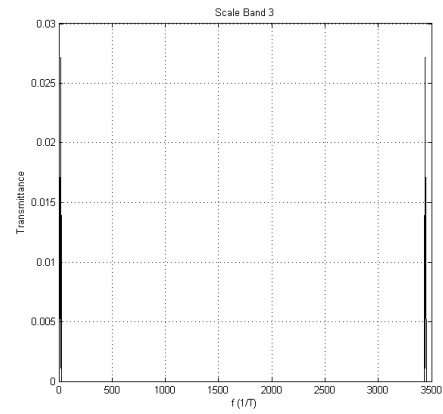
The absorption spectra can be considered as the original pulse processed by Fourier Transform. The horizontal coordinate should be wavenumber ( $\text{cm}^{-1}$ ), but as the data provided by the RIKEN record the value every 0.027 wavenumber ( $\text{cm}^{-1}$ ), we just enlarge the clearance value to 1. It means we stretch the horizontal coordinate about 37 times.

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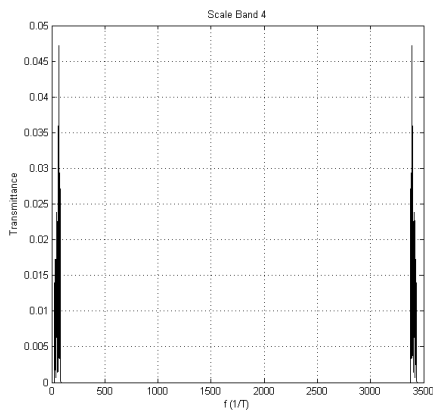
Wave atoms transform can represent a signal in different dimensions each scale band represents a portion of original spectrum for different frequency range. In our cases, there are 7 scale bands after applying wave atom transform to DASTSC. The number of scale band is dependent on the length of the input i.e. the number of points. For every scale



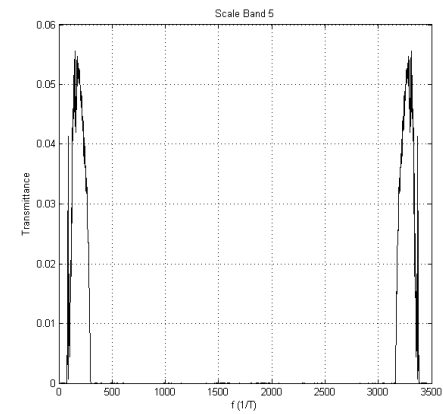
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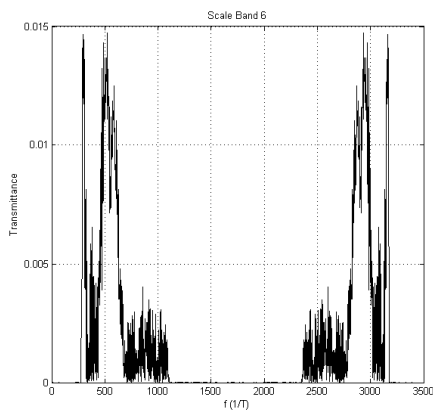
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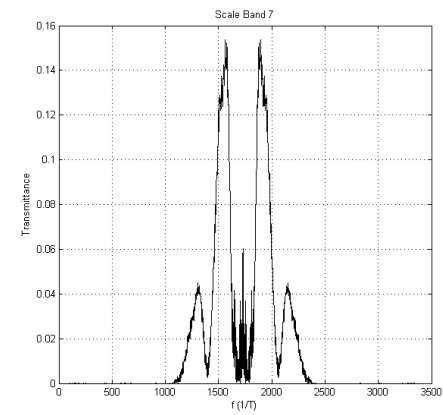
e



f



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h

Fig. 2 The spectrum of DASTSC and its 7 scale band

absolute values of all coefficients are taken for an easy observation. If all these scale bands are added together, the original spectrum can be obtained. The most significant outcome is found at the sixth scale band. If we observe the spectrum carefully, in Figure 3, we will find out the fifth scale

band represents the spectrum information between 700 and 1300Hz, while in Fourier Transformation (i.e. the original spectrum), it is very difficult to extract the signal information in these frequency range.

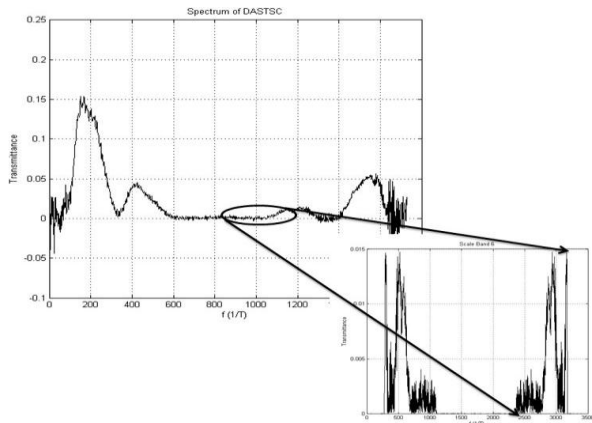


Fig. 3 The reconstruct signal of scale band 6 compared with the original spectrum

The reason behind is the peak values of spectrums in scale band 7 and scale band 5 are too large for it in band 5. In most situations, if we apply a filter to further refine the spectrum, the information in scale band 5 will be filtered. But in fact, there is a big chance that the fifth scale band may possess some optical properties of the testing material. In FFT, due to the effect of the some large pulses, some small signals are masked. By dividing the signal into different scale bands, it makes easier to analyze the data one by one. With using our method, a filter is applied to refine the spectrum, thereby keeping most of the masked signals. The Wave atoms transformation can divide a signal into different spectrums such as 6 to 8 scale bands where can explore some valuable information which is usually concealed by the main signal.

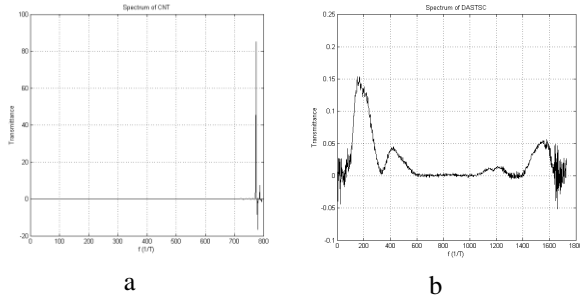


Fig. 4 Spectrum of CNT and DASTSC

By applying wave atoms transform, 70% test cases indicate that the resolution in the frequency domain has been improved. If we use Fourier Transform, there will be covered signals existing in these cases. According to the test results, we find that the proposed method is most suitable for analyzing the spectrums which have one or several distinct pulses. From the testing case CNT (single wall carbon nanotube) has one strong pulse at the end of the spectrum and DASTSC have 3 distinct wave crests (showing in Figure 4).

In these cases, the strong pulses cover up the other signals. It is hard to recover signal from the noises if using the traditional method. In addition, for a strong pulse, it has a big chance to appear in the last scale band according to the testing results. And in most cases, the covered signals are distributed

in 2 or 3 scales bands before the last band. The spectrums in these scale bands are usually appeared as sharp wave forms which can be easily distinguished from the noises. It is considered that these spectrums are generated by the reflection when the radiation goes through the substance. It helps us to further analyze the characteristics of the substance. Figure 5 shows that for the spectrums which are steadily decreasing, for these testing cases, the improvement in the spectrum are not significant.

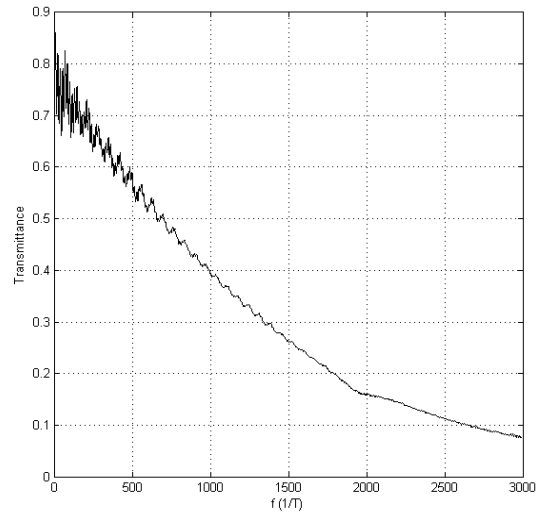


Fig. 5 A monotonic decreasing THz spectrum

It also shows a very interesting phenomenon from these test results. For the first 3 scale bands, almost all the test data show the same spectrums. There is a pulse point located at the edge. The above three test cases have already shown the situation. It is believed it is not a coincidence, which will be investigated in the future.

## V. CONCLUSIONS

In this paper, a new method of analyzing THz pulses based on wave atom transform is presented. It is considered that traditional Fourier Transform has a poor performance in the spectrum analysis of reflected/decayed oscillated waves. In recent research studies, it is found that wave atom transform is a powerful technique for analyzing signals which consist of oscillatory functions. Therefore, 1D wave atoms transform applied into the THz pulse analysis is introduced. The main idea is to decompose a signal into several spectrums with different frequency bands using wave atoms transform. In frequency domain, the resolution is improved where some reflected or decayed components which are concealed by the main pulse can be extracted into several bands for analyzing. By testing 50 spectrums, it is found that 72% of the spectrums which have obvious reflected/decayed components can be refined with wave atoms. If Fast Fourier transform is used instead, it has a big chance that some valuable information will be filtered out. Besides, it has been shown that that the

proposed method is most suitable for the spectrums which have one or several distinct wave crests, but for the spectrums which are monotonic decreasing, the improvement is not significant. To conclude, THz pulse analysis with wave atom outperforms conventional THz-TDS analysis methods

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