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Phase Function Effects on Identification of Terahertz Spectral Signatures Using the Discrete Wavelet Transform

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Abstract

We describe the application of the Discrete Wavelet Transform (DWT) in extracting the characteristic absorption signatures of materials from terahertz reflection spectra. We compare the performance of different mother wavelets, including Daubechies, Least Asymmetric (LA), and Coiflet, based on their phase and gain functions and filter lengths. We show that the phase functions of the wavelet and scaling filters result in spectral shifts to the absorption lines in the wavelet domain. We provide a solution by calculating advancement coefficients necessary to achieve effective zero-phase-function DWT. We demonstrate the utility of this signal processing technique using α -lactose monohydrate/polyethylene samples with different levels of rough surface scattering. In all cases, the DWT-based algorithm successfully extracts resonant signatures at 0.53 and 1.38 THz, even when they are obscured by the rough surface scattering effects. The DWT analysis with accompanying phase corrections can be utilized as a robust technique for material identification in non-destructive evaluation (NDE) using terahertz spectroscopy.

Index Terms—

Discrete wavelet transforms; phase function; rough surface scattering; spectral analysis; terahertz (THz); zero-phase transform

I. Introduction

Certain applications of terahertz time-domain spectroscopy (THz-TDS) in biomedical sensing [1], pharmaceutical industries [2], security screening [3], and chemical identification [4] rely on the recognition of unique resonant signatures in the dielectric functions of materials [5]. Many low-frequency vibrational and torsional motions of molecular systems have the same energies as radiations at terahertz frequencies (100 GHz – 10 THz) [6], [7].

Therefore, absorption signatures appear in the dielectric functions of many chemicals and biomolecules [8], [9]. Identification of the unique but weak THz signature modes can be challenging due to the heterogeneity of the samples, scattering and experimental noise. Surface roughness and particle granularity on the order of THz wavelengths ($30\text{ }\mu\text{m} - 3\text{ mm}$) diminish the signal to noise ratio (SNR) by distributing the radiation into random directions [10]. The presence of scattering enables robust detection schemes such as diffused off-specular spectroscopy [3], although it introduces spectral distortions that obscure the absorption features [11]–[13]. For example, surface roughness in the form of random height variations with a Gaussian distribution introduces an exponential frequency roll-off in the reflection amplitude spectrum [14], [15]. This frequency roll-off decreases the bandwidth and weakens the spectral signatures. Different approaches have been proposed to overcome the scattering effects on the THz spectrum. Averaging 1600 spatially uncorrelated transmission measurements of a sample improved the SNR due to the random distribution of the scatterers [16]. However, obtaining many measurements is time consuming and is not practical for samples with smaller surface areas. Cepstral filtering has been employed in both transmission and reflection THz-TDS to mitigate granular [17] and rough surface scattering [13]. In cepstral analysis, low-pass or band-pass Gaussian filters are applied to the Fourier transform of the derivative of the THz spectra. The techniques based on the band pass or low pass filtering of the Fourier domain spectra require *a priori* knowledge on the material absorption features, such as its spectral location, FWHM, spectral shape, and the scattering characteristics to choose the right pass band for the filters. In contrast, wavelet methods, which have also been used for mitigating the effects of rough surface and volume scattering in THz-TDS [18]–[21], are agnostic to the sample material information or scattering details and give access to the entire spectrum. Wavelet multiresolution analysis (MRA) was proposed for retrieval of α -lactose monohydrate resonant signature at 0.54 THz obscured by rough surface scattering [18]. It was shown that this absorption resonance can be separated from other noise-associated features caused by the random rough surface scattering in fine-scale maximal overlap discrete wavelet transform (MODWT) detail coefficients. An iterative reconstruction technique using discrete wavelet transform (DWT) detail sub-bands was proposed to estimate the scattering-induced baselines in THz transmission extinction spectra [19]. However, the identification of the material resonant features in the presence of random noise and quasi-ballistic scattering effects were not studied.

In this paper, we present a DWT-based algorithm to extract and identify material resonant features using THz-TDS reflection measurements in the wavelet domain. We also investigate the effects of the phase and gain functions and the filter lengths of different orthogonal mother wavelet filter families on extraction of terahertz spectral signatures. In the DWT pyramid algorithm, cascades of scaling and wavelet filters with non-zero phase functions result in shifts in the spectral location of the extracted features. We show that for orthogonal mother wavelets with approximately linear phase functions, advancing wavelet coefficients at each level by a predetermined factor compensates for these spectral shifts. We compute the number of required advances based on the phase function of the mother wavelets. We investigate the effectiveness of our method by applying DWT to the deconvolved amplitude spectrum of samples made of α -lactose monohydrate with smooth and rough surfaces. We

demonstrate that DWT with accompanying phase corrections is a robust technique in identification of characteristic resonant signatures in the presence of scattering effects. In contrast to the MODWT MRA algorithm, which requires the inverse transform operation back to the ‘signal domain’ [18], the DWT-based algorithm presented here performs the feature extraction in the ‘wavelet domain’. Therefore, the new technique allows for subsequent signal processing steps, such as de-noising [22], dimensionality reduction [23], and classification [24] to be applied to the correctly-aligned coefficients in the wavelet domain. Moreover, the DWT benefits from the lower computational complexity as compared to MODWT. The new DWT-based technique proposed here potentially can find applications in non-destructive evaluation and terahertz spectroscopy for identification of chemicals.

II. Materials and Methods

A. Sample Preparation

We prepared sample discs with smooth and rough surfaces. Samples were made by mixing α -lactose monohydrate (80% by weight) in ultra-fine high-density polyethylene powders (620XXF HDPE, Micro Powders, Inc., Tarrytown, NY, USA) and pressing the mixture under 3000 psi load for three hours, which yielded 2mm-thick pellets with 50 mm diameter. HDPE was added as a binding agent and its THz spectrum is void of resonant signatures. Surface roughness was imprinted using 80-grit and 40-grit sandpapers (Norton Abrasives, Worcester, MA, USA) during the pellet pressing. Table I provides the statistics of the sandpaper sheets roughness including their average particle size, RMS height and correlation length. Fig. 1 illustrates the microscopic images taken from the surface of the pellets with smooth and rough surfaces by an optical microscope.

B. Measurement Setup

Reflection THz-TDS measurements were obtained using a TERA-ASOPS high-speed THz time-domain spectrometer (Menlo Systems, Inc., Newton, NJ, USA). TERA-ASOPS uses the difference in the repetition rates of two 1560 nm femtosecond lasers to scan the THz pulses at high rates. Laser pulses were guided by optical fibers to the emitter and detector photoconductive antenna (PCA) producing signals with 0.2 – 1.5 THz useful spectral range. Two TPX50 lenses (Menlo Systems, Inc., Newton, NJ, USA) collimated and focused the generated THz beams on the sample surface with angle of incidence $\theta_i = 36^\circ$, and focal spot size of approximately 4.7 mm. Similar lenses collimated and refocused the specular reflection beams on the THz detector. The smooth-surface sample position was adjusted so that signals reflected from the reference mirror were approximately aligned with the signals reflected from the surface of the sample. However, due to variations in the surface height of the 80-grit and 40-grit rough samples, the time of arrival varies for uncorrelated measurement spots. For each sample, 10 spatially disjoint measurements were deconvolved in the Fourier domain by a reflection from a reference mirror and their averaged amplitude spectrum was used in the following signal processing steps.

C. Signal Conditioning

Based on the Kirchhoff approximation, Gaussian surface variations with standard deviation σ , introduce a Gaussian decline in the coherent reflectivity [27]. With incident angles close

to the surface normal, reflected power is proportional to coherent reflectivity, P_{coh} given by [27], [28],

$$P(f) \propto P_{coh} e^{-4\kappa^2 \sigma^2 \cos^2 \theta_i}, \quad (1)$$

where κ is the wavenumber, and θ_i is the angle of incidence. Our measurements confirm the Gaussian decline in the rough-surface sample spectral amplitude. Fig. 2(a) compares the time-domain trace of the reflection from a smooth-surface sample, with that of an 80-grit and a 40-grit rough-surface sample. Surface roughness has resulted in significant drops in the SNR. Fig. 2(b) illustrates the scattering effects in the Fourier domain. Amplitude spectrum of the smooth-surface sample has a linear trend with a close-to-zero slope. Rough-surface samples' amplitude spectra demonstrate Gaussian frequency roll-offs, according to (1), which were numerically fitted to the measurements. Scattering has obscured the resonant features and as wavelength decreases the effects of scattering become more severe. Prior to wavelet transform, we detrended each spectral amplitude using its fitted profile, shown in Fig. 2(b). After detrending, we tapered the boundaries of each spectral signal by applying halves of a Hann window to each end of the spectrum. After zero-padding each N -point-length signal to $2^{J_0} \lceil N/2^{J_0} \rceil$, we applied the DWT for $J_0 = 8$ levels of decomposition using various mother wavelets.

D. Implementation of DWT Using the Pyramid Algorithm

A level J_0 DWT decomposes a signal into J_0 levels of scaling and wavelet coefficients by successively convolving it with a low-pass scaling filter, $g(f)$, and a high-pass wavelet filter, $h(f)$, using the pyramid algorithm shown in Fig. 3 [25], [26]. At each level, outputs of the filters are subsampled by a factor of 2. Filtering the signal with non-zero phase function wavelet and scaling filters and subsampling their outputs by 2 result in complicated misalignments between the original THz spectrum and the wavelet coefficients. At the higher levels with $j \geq 2$, cascades of the filters shown in Fig. 3 can be replaced by the aggregate filters $g_j(f)$ and $h_j(f)$. Here, $g_j(f)$ is formed by the convolution of scaling filters built upon up-sampling of $g(f)$ by 2^a for $a = 0, 1, \dots, j-1$. Also, $h_j(f)$ is formed similar to $g_j(f)$ except that $g(f)$ is replaced by $h(f)$ at $a = j-1$. Taking sub-samplings into account, $W_j(f)$ is given by,

$$W_j(f) = \sum_{l=0}^{L_j-1} h_j(l) X(2^j(f+1) - 1 - l \bmod N), \quad (2)$$

and $V_j(f)$ is given by,

$$V_j(f) = \sum_{l=0}^{L_j-1} g_j(l) X(2^j(f+1) - 1 - l \bmod N). \quad (3)$$

L_j represents the length of the aggregate filters and is computed based on the length of the mother wavelet filter, $\mathcal{L}$, as

$$L_j = (2^j - 1)(\mathcal{L} - 1) + 1. \quad (4)$$

We compute the phase functions of $g(f)$ and $h(f)$ for three well-known orthogonal wavelet families namely Daubechies $D(\mathcal{L})$, Least Asymmetric $LA(\mathcal{L})$, and Coiflet $C(\mathcal{L})$. In [29], Daubechies proposes a few classes of orthogonal wavelet filters that yield wavelet coefficients associated with the differences of the adjacent weighted averages of a signal. These wavelet filter families, including $D(\mathcal{L})$ and $LA(\mathcal{L})$, share the same squared gain function (squared Fourier amplitude) while their phase function characteristics are different. $D(\mathcal{L})$ is defined to have minimum delay or extremal phase, whereas $LA(\mathcal{L})$ is defined to have the highest symmetry, least asymmetry, or equivalently highest phase function linearity among the filters that satisfy the same gain function. In contrast to $D(\mathcal{L})$ and $LA(\mathcal{L})$ filters, $C(\mathcal{L})$ squared gain function is different such that it yields higher phase function linearity. However, $C(\mathcal{L})$'s better phase function characteristics come at the cost that it produces artificial triangular-shape artifacts in the wavelet coefficients. Here we investigate how the phase and gain function properties of orthogonal wavelets defined in [29] affect the extracted THz resonant features. The method described here to remove the spectral shifts can be generalized to other mother wavelet families. Fig. 4(a) shows the baseline subtracted average amplitude spectrum of the smooth-surface sample. We took its DWT using $C(6)$, $D(6)$, $LA(8)$ and $LA(12)$ mother wavelets for $J_0 = 8$ levels of decomposition. Vertically offset normalized 5th level wavelet coefficients, $W_5(f)$, are shown in Fig. 4(b), as an example. The plotted wavelet coefficients extract the resonant signatures as sharp easily distinguishable features. They extract both α -lactose monohydrate and ambient water vapor absorption resonances which are shown using the vertical dashed lines in Fig 4(a). By zooming into the wavelet coefficients at 0.54 THz, in Fig 4(c), and 1.39 THz, in Fig. 4(d), the misalignments between the wavelet coefficients and the expected location of absorption features are demonstrated. In the following section, we will investigate the cause of the misalignments theoretically, and calculate advancement compensation factors to correct the location of the extracted spectral features.

E. Zero-Phase DWT

The phase function of a scaling or a wavelet filter can be obtained using the phase of the Fourier transform of each filter. To avoid confusion between the frequency in the Fourier domain (used for THz spectral data) and the Fourier transform of the scaling and wavelet filters, we represent the latter in terms of discrete frequency k . Fig. 5(a) illustrates the phase function of the 1st level $LA(8)$ scaling filter along with the three closest linear phase approximations, $-4\pi k$, $-6\pi k$, and $-8\pi k$. Among these three, $g(f)$ phase function, $\theta_{LA(8)}^g(k)$, demonstrates the least deviations from $-6\pi k$. Therefore, it can be approximated to be a linear function of k , with an advancement factor ν ,

$$\theta_{LA(8)}^g(k) \approx 2\pi k\nu; \nu = -3. \quad (5)$$

Phase function of a wavelet filter, $h(f)$, defined to be the quadrature mirror filter (QMF) of the scaling filter given by,

$$h(f) = (-1)^f g(\mathcal{L} - 1 - f), \quad (6)$$

is calculated by [25],

$$\theta^h(k) = -(2\pi k(\mathcal{L} - 1) - \pi) + \theta^g\left(\frac{1}{2} - k\right). \quad (7)$$

For the LA(8) wavelet filter, (5) and (7) imply that

$$\theta_{LA(8)}^h(k) \approx -2\pi k(\mathcal{L} - 1 + \nu) + \pi(\nu + 1). \quad (8)$$

Here, (8) represents a linear phase function only for odd values of ν . Because ν given by (8) for $\theta_{LA(8)}^g(k)$, the scaling filter, is an odd value, its corresponding wavelet filter will have a linear phase function too. To verify this, Fig. 5(b) illustrates the phase function of the 1st level LA(8) wavelet filter along with the three closest linear phase approximations, $-6\pi k$, $-8\pi k$, and $-10\pi k$. It can be seen that $\theta_{LA(8)}^h(k)$ demonstrates the least deviations from $-8\pi k$. Therefore, it follows (8) by setting $\nu = -3$ and $\mathcal{L} = 8$. We can generalize (5) and (8) to other LA($\mathcal{L}$) mother wavelets. In other words, if the phase function of a LA($\mathcal{L}$) scaling filter is approximately linear and given by $2\pi k\nu$, for an odd value of ν , the phase function of its wavelet filter will also be approximately linear and given by $-2\pi k(\mathcal{L} - 1 + \nu)$. Indeed, ν is always odd for $\{LA(\mathcal{L}): \mathcal{L} = 8, 10, \dots, 20\}$ mother wavelets and is specified by $\mathcal{L}$ using [25], [30],

$$\nu_{LA(\mathcal{L})} = \begin{cases} -\mathcal{L}/2 + 1 & \mathcal{L} = 8, 12, 16, 20; \\ -\mathcal{L}/2 & \mathcal{L} = 10, 18; \\ -\mathcal{L}/2 + 2 & \mathcal{L} = 14. \end{cases} \quad (9)$$

Advancing the 1st level LA(8) scaling and wavelet filters by $|\nu|$ and $|\mathcal{L} - 1 + \nu|$ units, respectively, results in approximate zero-phase filters at the 1st level of the pyramid algorithm. At the higher levels, $j \geq 2$, we need to find the phase functions of $g_j(f)$ and $h_j(f)$. Transfer function of $g_j(f)$, which is formed by the convolution of up-sampled 1st level scaling filters, is given by,

$$G_j(k) = \prod_{a=0}^{j-1} G(2^a k). \quad (10)$$

Therefore, the phase function of $g_j(f)$ can be calculated by the summation of the phase of the transfer functions in (10) using,

$$\theta_j^g(k) = \sum_{a=0}^{j-1} \theta^g(2^a k). \quad (11)$$

For LA($\mathcal{L}$) scaling filters, (5) and (11) yield

$$\theta_{LA(\mathcal{L})}^{g_j}(k) = \sum_{a=0}^{j-1} 2\pi(2^a k)\nu = 2\pi k\nu(2^j - 1), \quad (12)$$

which is a linear phase function with $\nu^{g_j} = \nu(2^j - 1)$. Similar to $g_j(f)$, transfer function of $h_j(f)$, which is formed by the convolution of the up-sampled 1st level scaling and wavelet filters, is given by,

$$H_j(k) = H(2^{j-1}k) \prod_{a=0}^{j-2} G(2^a k). \quad (13)$$

Therefore, phase function of $h_j(f)$ will be formed by the summation of the phase of the transfer functions in (13) using,

$$\theta_{h_j}^j(k) = \theta^h(2^{j-1}k) + \sum_{a=0}^{j-2} \theta^g(2^a k). \quad (14)$$

For LA($\mathcal{L}$) wavelet filters, using (5) and (8) in (14) results in

$$\theta_{LA(\mathcal{L})}^{h_j}(k) = 2\pi k(-2^{j-1}(\mathcal{L} - 1) - \nu). \quad (15)$$

It can be noted that (15) is also a linear phase function with an advancement factor $\nu^{h_j} = -2^{j-1}(\mathcal{L} - 1) - \nu$. Therefore, advancing $g_j(f)$ and $h_j(f)$ of LA($\mathcal{L}$) mother wavelets by respectively $|\nu^{g_j}|$ and $|\nu^{h_j}|$ units results in a zero-phase filtering at the j^{th} level of the DWT. Similar results are valid for C($\mathcal{L}$) mother wavelets except that it can be shown that their ν values are different and set by [25],

$$\nu = -\frac{2\mathcal{L}}{3} + 1. \quad (16)$$

Fig. 6(a) illustrates that the phase function of the C(6) scaling filter has the least deviations from $-6\pi k$. This can be verified by setting $\mathcal{L} = 6$ in (16) and using it in (12) for $j = 1$. Fig. 6(b) demonstrates that the C(6) wavelet filter phase function has the least deviations from $-4\pi k$. This result also can be obtained by setting $\mathcal{L} = 6$ in (16) and using it in (15) for $j = 1$. Phase functions of the higher-level C(6) wavelet and scaling filters, $j \geq 2$, can be calculated in a similar way using (12) and (15).

Fig. 7 illustrates the phase functions of the 1st level D(4) wavelet and scaling filters along with their linear phase approximations. It can be noted that differences between the phase functions of D(4) filters and the closest linear phase approximations are larger than those of the LA(8) and C(6), which demonstrates D(4)'s higher non-linearity.

To evaluate the effects of the circular advances on the phase functions, Fig. 8 compares the phase functions of the advanced wavelet filters, $h_j(f)$ for $j = 1, \dots, 4$, of different mother wavelets. Number of advances for LA(8) and C(6) mother wavelets are set using (9), (15)

and (16). For comparison to wavelet filters with non-linear phase functions, D(4) wavelet filter also was advanced using (15). Although the phase function of the 1st level D(4) wavelet filter is non-linear, because it demonstrates the least deviations from $-4\pi k$, we used $\nu = -2$ for D(4) wavelet filters. In Fig. 8, phase functions of the advanced wavelet filters are shown in their respective pass-bands, which depend on j and are given by $\frac{1}{2^{j+1}} \leq |k| \leq \frac{1}{2^j}$.

These pass-bands are separated by the vertical dashed lines. Phase functions of the advanced C(6) wavelet filters are closer to zero than LA(8) and D(4). Advancing the D(4) wavelet filters does not yield zero-phase filters. This corresponds to the non-linearity of the D(4) phase functions.

Noteworthy here, because of the sub-samplings by 2^j , advancing the filters coefficients does not suffice to correct the misalignments in DWT outputs. Without sub-sampling, advancing a $h_j(f)$ by $\lfloor \nu^{hj} \rfloor$ units in (2) yields,

$$\sum_{l=0}^{L_j-1} h_j(l + \lfloor \nu^{hj} \rfloor) X(f - l \bmod N) = \widetilde{W}_j(f + \lfloor \nu^{hj} \rfloor \bmod N), \quad (17)$$

where $\widetilde{W}_j$ represents un-sampled wavelet coefficients. Here, (17) implies that for zero-phase filtering, without sub-sampling, we must associate the original signal, $X(f)$, with $\widetilde{W}_j(f + \lfloor \nu^{hj} \rfloor \bmod N)$ or likewise $X(f - \lfloor \nu^{hj} \rfloor \bmod N)$, $X(f)$ delayed by $\lfloor \nu^{hj} \rfloor$ units, with $\widetilde{W}_j(f)$. Now, Sub-sampling $\widetilde{W}_j(f)$ by 2^j yields DWT wavelet coefficients as

$$W_j(f) = \widetilde{W}_j(2^j(f+1)-1). \quad (18)$$

Therefore, associating $\widetilde{W}_j(f)$ with $X(f - \lfloor \nu^{hj} \rfloor \bmod N)$ results in the association of $W_j(f)$ with $X(2^j(f+1)-1 - \lfloor \nu^{hj} \rfloor \bmod N)$. For example, for the 2nd level C(6) wavelet coefficients with $\lfloor \nu^{h2} \rfloor = 7$, $W_j(0)$ should be plotted against $X(N-4)$, the $(N-4)$ th data point in $X(f)$. To find the right order of DWT wavelet coefficients, we find a f_0 such that $W_j(f_0)$ aligns with $X(0)$ and advance $W_j(f)$ by f_0 . By setting the argument of $X(2^j(f_0+1)-1 - \lfloor \nu^{hj} \rfloor \bmod N)$ to zero we will have

$$f_0 = \left\lceil \frac{1 + \lfloor \nu^{hj} \rfloor}{2^j} - 1 \right\rceil. \quad (19)$$

The flow chart in Fig. 9 summarizes the signal processing steps required for the correct identification of THz resonant signatures using DWT.

III. Results and Discussion

A. Smooth-surface Sample Results

Fig. 10 illustrates the results of advancing the 3rd to 5th level wavelet coefficients of the deconvolved smooth-surface sample amplitude spectrum. Wavelet coefficients were obtained

using the C(6), D(6), LA(8), and LA(12) mother wavelets. The numbers of applied advances obtained using (19) are shown in the powers of T , i.e. $T^{-f_0}W_j$, next to each mother wavelet results. In Fig. 10(b), C(6) wavelet coefficients perform better in extracting the resonant signature at 0.54 THz in comparison to other mother wavelets. Moreover, as filter length $\mathcal{L}$ increases, the extracted features become sharper and the scattering effects are suppressed. To explain these observations, we compare the gain functions of the 3rd level C(6), D(6), LA(8), and LA(12) wavelet filters in Fig. 11. Fig. 11 illustrates that as the filter length increases, the side-lobes of the gain functions become smaller, and the main pass-band given by $\frac{1}{16} \leq k \leq \frac{1}{8}$ is narrower. This change in the gain function results in the wavelet filters with smaller lengths to allow more low-frequency content, which appear as noisy fluctuations in the entire spectrum. Because the absorption signature of α -lactose monohydrate at 0.54 THz is a broader feature compared to the other resonant signatures, it has a more significant low-frequency content. Here, by the frequency content of a spectral signature, we refer to the Fourier transform of the THz spectral data. In other words, it is a function of k . Because C(6) wavelet filter gain function covers more lower frequencies, 0.54 THz feature is larger in its wavelet coefficient outputs. On the other hand, larger side-lobes allow more noisy fluctuations into the outputs of C(6) as well. Similar conclusions are valid for the 4th and the 5th level wavelet coefficients shown in Fig. 10(c) and Fig. 10(d). Finally, although the 0.54 THz signature is hardly distinguishable in the 3rd level LA(8) and LA(12) wavelet coefficients, as j increases, the resonant feature gets larger and clearer. Fig. 12 shows the gain functions of the 3rd to 5th level LA(12) wavelet filters. It illustrates that as j increases, the wavelet filter pass-band moves toward lower k frequencies. Therefore, 0.54 THz signature becomes larger in the output. Besides, increasing j makes the filter pass-band narrower, and therefore, it allows less amount of low-frequency fluctuations into its outputs. To compare the effectiveness of the proposed advancements in correcting the phase distortions, α -lactose monohydrate signatures at 0.54 THz and 1.39 THz are slightly misaligned in the outputs of D(6) in Fig. 10(b) and Fig. 10(c). However, C(6), LA(8), and LA(12) outputs are all perfectly aligned with the input. This is because of the non-linear phase function of the D(6) wavelet filters. Table II provides the explicit locations of the extracted resonances at each level before and after the circular advancements. Noteworthy here, applying an amplitude-based thresholding scheme to the baseline-subtracted signal shown in Fig. 10(a) results in omission of the α -lactose monohydrate resonance at 1.21 THz, and water vapor resonances at 1.09 THz and 1.16 THz. Additionally, it might also account for the 0.2 THz feature, which is caused by the low-frequency noise, as a resonant signature.

B. Rough-surface Sample Results

The RMS surface height that can result in significant levels of rough surface scattering is determined using the Fraunhofer criterion, given by [27],

$$h \geq \frac{\lambda}{32\cos\theta_i}, \quad (20)$$

where λ is the wavelength and θ_i is the incident angle. At $\theta_i = 36^\circ$, 80-grit and 40-grit sandpapers give rise to significant scattering at $f = 0.21$ THz and $f = 0.08$ THz, respectively.

Therefore, for the rough-surface samples, all the resonant features are affected by scattering effects. Fig. 13 shows the DWT wavelet coefficients of the rough-surface sample amplitude spectrum. Fig. 13(a) illustrates the base-line subtracted deconvolved amplitude spectrum averaged over 10 spatially disjoint measurements. The resonant signatures at 1.09 THz, 1.16 THz and 1.21 THz of the signal shown in Fig. 13(a) are hardly distinguishable and an amplitude thresholding scheme is unable to detect them. The advanced 4th level wavelet coefficients using C(6), D(6), and LA(8) mother wavelets are shown in Fig. 13(b). Wavelet coefficients were able to extract even the obscured water absorption lines between 1.1 and 1.25 THz. However, the noisy fluctuations surrounding these features are more prominent in comparison to the smooth-surface sample results. These fluctuations, which are mostly due to the noise and scattering effects, make the recognition of resonant features more challenging. However, as we explained in Fig. 11, when the filter length increases, it would allow less low-frequency fluctuations. To investigate the effects of the filter length on the rough-surface sample wavelet coefficients, we used C(12), D(12), and LA(12) wavelets in Fig. 14. Fig. 14(b) illustrates the 4th level wavelet coefficients advanced by the values obtained by (19). In comparison to Fig. 13, noise levels are greatly suppressed, and the resonant features are more clear. Here, C(12) and LA(12) results also make perfect alignment with the input, whereas D(12) advanced coefficients are still slightly misaligned. Table III provides the explicit locations of the extracted resonances of the 80-grit rough sample at each level before and after the circular advancements.

To further investigate the robustness of the DWT in extracting the THz resonant features, we applied it with the accompanying phase function corrections to 40-grit rough sample. Fig. 15 compares the 4th level wavelet coefficients of the smooth-surface sample with those of the 80-grit and 40-grit rough samples. Although noise-associated features are prominent in 40-grit results, the material resonant features are still clearly discernible. In particular, LA(8) and LA(12) are successful in suppressing the scattering effects. Comparing the results of both smooth-surface and rough-surface samples reveals that LA(8) and C(12) are more suitable choices for THz resonance extraction. They both can extract all the resonant features simultaneously. They have narrower pass-bands and therefore can eliminate the low- k -frequency scattering effects. Finally, advancing their coefficients results in effective zero-phase filters without causing any phase distortions.

IV. Conclusion

We used the DWT for extracting resonant signatures from deconvolved amplitude spectrum of THz signals reflected from sample pellets with smooth and rough surfaces. We showed that although the resonant signatures are obscured by scattering effects, the DWT wavelet coefficients identify them as sharp and easily distinguishable features. We also investigated the effects of the phase function of the wavelet and scaling filters on the location of the extracted resonances. We provided phase function corrections in the form of advancing output wavelet coefficients at each scale. Therefore, we achieved zero-phase filtering and exact alignment of extracted resonances. We also compared the phase and gain functions of different mother wavelets. The LA($\mathcal{L}$) and C($\mathcal{L}$) could create larger spectral shifts, however due to their linear phase functions, advancing filter coefficients will result in effective zero-phase filters. In contrast, despite causing less spectral shifts, the phase function of D($\mathcal{L}$)

cannot give a zero-phase transform after advancement compensation. Our results showed that this behavior of $D(\mathcal{L})$ family of wavelets is attributed to the high nonlinearity of their phase functions. We also compared mother wavelets of various lengths and showed that as the length of the filter increases, it suppresses more low- k -frequency content (broader features), which results in wavelet coefficients revealing sharp resonances such as water vapor absorption lines. Therefore, to extract broader resonances, like α -lactose monohydrate signature at 0.54 THz, mother wavelets with smaller lengths should be used. Based on phase and gain functions characteristics, the LA(8) and C(12) are reasonable choices for extracting both water and α -lactose monohydrate resonances from smooth and rough-surface samples simultaneously. In comparison to the MODWT [18], the main benefit of zero-phase DWT is that it allows for continuation of subsequent signal processing steps in the wavelet domain. MODWT often results in larger spectral shifts in the wavelet domain and can yield zero-phase filtering only after transforming the signal back to the frequency domain - also known as the multiresolution analysis (MRA). Noteworthy here, the same approach explained in this work for zero-phase DWT using orthogonal mother wavelets is also applicable for DWT with biorthogonal family of wavelets. In biorthogonal wavelets, the phase function of the employed wavelet and scaling filters are deterministically linear, and therefore approximations made in this paper are not necessary. Future works include investigating the sensitivity and specificity of wavelet transform in identification of resonant signatures.

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Biographies

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Fig. 1. Microscopic images (2.5 x) of the surface of the sample discs with (a) smooth surface, (b) 80-grit rough surface and (c) 40-grit rough surface.

Fig. 2.

(a) Specular THz-TDS signals reflected off smooth-surface, 80-grit and 40-grit rough-surface α -lactose monohydrate samples, (b) spectral amplitude of 10 spatially disjoint measurements taken from each sample and deconvolved by a reflection from a reference mirror. Each sample amplitude spectrum was numerically fitted to (1) for spectral detrending (dotted dashed lines).

Fig. 3.

The block diagram of the pyramid algorithm of a partial DWT of level J_0 . $X(f)$ is the input spectral signal. $h(f)$ and $g(f)$ represent the first level DWT wavelet and scaling filters, respectively. Outputs of each filter are subsampled by 2. $W_j(f)$ are the j^{th} level wavelet coefficients and $V_{J_0}(f)$ are the J_0^{th} level scaling coefficients.

Fig. 4.

(a) Base-line subtracted average amplitude spectrum of the smooth-surface sample, (b) vertically offset normalized 5th level DWT wavelet coefficients of signal in (a) using C(6), D(6), LA(8), and LA(12) mother wavelets, (c) $W_5(f)$ in the range 0.45 – 0.65 THz, (d) $W_5(f)$ in the range 1.3 – 1.5 THz. Vertical dashed lines delineate the correct positions of the resonant signatures.

Fig. 5.

(a) Phase function of the 1st level LA(8) scaling filter, $g(f)$, along with the closest linear phase approximations. The inset shows the difference between $\theta_{LA(8)}^g(k)$ and $-6\pi k$, from which $\theta_{LA(8)}^g(k)$ has the least deviations, (b) phase function of the 1st level LA(8) wavelet filter, $h(f)$, along with the closest linear phase approximations. The inset shows the difference between $\theta_{LA(8)}^h(k)$ and $-8\pi k$, the closest approximation to $\theta_{LA(8)}^h(k)$.

Fig. 6.

(a) Phase function of the 1st level C(6) scaling filter, $g(f)$, along with the closest linear phase approximation. Inset shows the difference between $\theta_{C(6)}^g(k)$ and $-6\pi k$, from which $\theta_{C(6)}^g(k)$ has the least deviations, (c) phase function of the 1st level C(6) wavelet filter, $h(f)$, along with the closest linear phase approximations. Inset shows the difference between $\theta_{C(6)}^h(k)$ and $-4\pi k$, from which $\theta_{C(6)}^h(k)$ has the least deviations.

Fig. 7.

(a) Phase function of the 1st level D(4) scaling filter, $g(f)$, along with the closest linear phase approximation. Inset shows the difference between $\theta^g_{D(4)}(k)$ and $-2\pi k$, from which $\theta^g_{D(4)}(k)$ has the least deviations, (b) phase function of the 1st level D(4) wavelet filter, $h(f)$, along with the closest linear phase approximations. Inset shows the difference between $\theta^h_{D(4)}(k)$ and $-4\pi k$, from which $\theta^h_{D(4)}(k)$ has the least deviations.

Fig. 8.

Phase functions of the advanced LA(8), C(6) and D(4) wavelet filters: $h_j(f)$: $j = 1, \dots, 4$.

Phase function of j^{th} level wavelet filter is plotted against its pass band given by

$$\frac{1}{2^{j+1}} \leq k \leq \frac{1}{2^j}.$$

Fig. 9.

Flowchart presents the signal processing steps for implementation of DWT in extraction of resonant signatures in the terahertz reflection spectra.

Fig. 10.

(a) Base-line subtracted average amplitude spectrum of the smooth-surface sample, (b) advanced $W_3(f)$, (c) advanced $W_4(f)$, (d) advanced $W_5(f)$. C(6), D(6), LA(8), and LA(12) mother wavelets were used. Number of advances obtained using (19) are shown in the powers of T , $T^{-f_0}W_j$. Blue and red sub-plots at each level zoom into the advanced wavelet coefficients at 0.54 THz and 1.39 THz, respectively. Vertical dashed lines delineate the correct positions of the resonant signatures.

Fig. 11.

Gain functions of the 3rd level C(6), D(6), LA(8), and LA(12) wavelet filters. As filter length, $\mathcal{L}$, increases, filter sidelobes get smaller and its pass-band gets narrower around $\frac{1}{16} \leq k \leq \frac{1}{8}$.

Fig. 12.

Gain function of the 3rd to 5th level LA(12) wavelet filters. Increasing the j makes the pass band of the filter narrower and containing smaller frequencies.

Fig. 13.

(a) Base-line subtracted average deconvolved amplitude spectrum of an 80-grit rough-surface sample made of α -lactose monohydrate and HDPE, (b) advanced 4th level wavelet coefficients of the signal in (a) obtained using C(6), D(6), and LA(8) mother wavelets. Blue and red sub-plots zoom into the wavelet coefficients at 0.54 THz and 1.39 THz. Vertical dashed lines delineate the correct positions of the resonant signatures.

Fig. 14.

(a) Base-line subtracted average deconvolved amplitude spectrum of an 80-grit rough-surface sample made of α -lactose monohydrate and HDPE, (b) advanced 4th level wavelet coefficients of the signal in (a) obtained using C(12), D(12), and LA(12) mother wavelets. Blue and red subplots zoom into the wavelet coefficients at 0.54 THz and 1.39 THz. Vertical dashed lines delineate the correct position of the resonant signatures.

Fig. 15.

The advanced 4th level DWT wavelet coefficients of the smooth, 80-grit, and 40-grit rough samples detrended amplitude spectra using (a) C(6), (b) D(6), (c) LA(8), and (d) LA(12) mother wavelets.

TABLE I

Statistical Parameters for Rough Surface Characterization of 80 Grit and 40 Grit Sandpapers

Grit	Average Particle Size (μm)	RMS Height (μm)	correlation Length (μm)
80	190	55	151
40	425	135	420

TABLE II

Peak Positions for the Smooth Sample Before and After Phase Shifts

		0.54 THz		1.21 THz		1.39 THz	
		W_j	TW_j	W_j	TW_j	W_j	TW_j
C(6)	$j=3$	0.56	0.54	1.22	1.21	1.41	1.39
	$j=4$	0.56	0.54	1.23	1.21	1.41	1.39
	$j=5$	0.57	0.53	1.24	1.20	1.43	1.39
D(6)	$j=3$	0.56	0.55	1.23	1.22	1.41	1.39
	$j=4$	0.57	0.55	1.24	1.22	1.42	1.40
	$j=5$	0.59	0.55	1.24	1.20	1.43	1.39
LA(8)	$j=3$	0.56	0.54	1.23	1.21	1.41	1.39
	$j=4$	0.57	0.54	1.24	1.21	1.42	1.39
	$j=5$	0.59	0.53	1.26	1.2	1.45	1.39
LA(12)	$j=3$	0.57	0.54	1.24	1.22	1.42	1.39
	$j=4$	0.59	0.54	1.26	1.21	1.44	1.39
	$j=5$	0.63	0.53	1.30	1.20	1.49	1.39

TABLE III

Peak Positions for the 80-Grit Rough Sample Before and After Phase Shifts

	0.54 THz		1.21 THz		1.39 THz	
	w_4	$T^{-f_0}W_4$	w_4	$T^{-f_0}W_4$	w_4	$T^{-f_0}W_4$
C(6)	0.56	0.54	1.23	1.21	1.42	1.39
D(6)	0.57	0.55	1.24	1.22	1.42	1.39
LA(8)	0.57	0.54	1.24	1.21	1.43	1.39
C(12)	0.59	0.54	1.26	1.21	1.45	1.39
D(12)	0.58	0.53	1.25	1.20	1.44	1.38
LA(12)	0.59	0.54	1.26	1.21	1.45	1.39