A 3-Dimensional display and process software for THz spectrum

Xiaowen Jiang\(^1\), Zhaohui Zhang\(^1\), Xiaoyan Zhao\(^1\), Yixin Yin\(^1\), Katsuhiro Ajito\(^2\) and Hojin Song\(^2\)

\(^1\) Information Engineering School, University of Science and Technology Beijing, Beijing 100083, China
\(^2\) NTT Basic Research Laboratories, Kanagawa243-0198, Japan

E-mail: zhangzhaohui@ustb.edu.cn

**Abstract.** An underpinning software is devoted to THz spectrum analyzing and 3-D imaging. The paper describes the software’s outline, structure, functions and some of considerations. Users in LAN (local area network) can access it and implement some basic and advanced works such as files operation, echoes cutting, spectrum calculation, baseline cancelling, peak fitting, qualitative and quantitative measuring of solid-state samples.

1. **Introduction**
Terahertz sensing and imaging technologies [1] push massive data to us, and we hardly make use of them without specific software. This paper describes a software package for THz spectrum process, in which the primary data can be transferred to absorbance or transmittance spectra at any pixel of a pellet sample surface, and 3D images can be shown with messages of concentration distributions. Several algorithms, such as baseline fitting, peak fitting, and substance identifying and quantitative measuring of mixture are involved.

2. **Remote login**
The software bases on Java Web. Figure 1 shows that users in LAN can login, and upload files to or download files from a Tomcat server where the software runs.

![Figure 1. Interface after login](image)

3. **Data process for a pixel**
3.1. Echo cutting

As both sides of a solid-state sample resulting in incident reflection, the acquired waveform data need preprocessing to eliminate echoes and extract the essential part of them. The schematic diagram of cutting echoes from $E_{sam}(t)$ and $E_{ref}(t)$ which are time-resolved data of the sample and the reference correspondingly[2, 3], is shown in figure 2.

![Schematic diagram of cutting echoes](image)

**Figure 2.** Procedures of echo cutting

3.2. Absorbance and transmittance spectra

Denote the time-resolved electric fields of a sample and a reference as $E_{sam\_cut}(t)$ and $E_{air\_cut}(t)$ after echo cutting, and their Fourier transformations as $E_{sam}(\omega)$ and $E_{ref}(\omega)$. Based on Duvillare’s theory[2], the absorbance spectra $\alpha(\omega)$ is calculated as following.

$$\alpha(\omega) = -\frac{2}{d} \ln \left[ \frac{|E_{sam}(\omega)|}{|E_{ref}(\omega)|} \frac{[n_s(\omega) + 1]^2}{4n_s(\omega)} \right]$$

(1)

Where $d$ is the sample’s thickness; $n_s(\omega)$ is its refractive index. Similarly, the transmittance spectrum is as following:

![Spectra](image)

**Figure 3.** Spectra carried out from formulas
(a) absorbance spectra; (b) transmittance spectra
\[ T(\omega) = \left( \frac{E_{\text{ref}}(\omega)}{E_{\text{sum}}(\omega)} \right) \left( \frac{4n_0(\omega)}{n_0(\omega) + 1} \right)^{\frac{2}{3}} \]  

(2)

See figures 3(a) and 3(b). Both of them exhibit specific peaks [4], but the former baseline is rising while the later is declining as increasing frequencies. That’s reasonable because absorbance is always against transmittance.

3.3. Spectrum baseline fitting and removing

Figure 4. Baseline fitting. (a) absorbance baseline fitting; (b) transmittance baseline fitting

Figure 5. Spectra with removing baselines. (a) absorbance spectra; (b) transmittance spectra

Spectrum baselines come from scattering of incident light by sample’s granules. In order to analyze absorbing or transmitting phenomena without disturbance, the baselines should be removed. In figure 3, the baseline can be regarded as an exponential (blue curve) or polynomial (red curve) function of frequency. The baseline then should be fit by an exponential or polynomial function as following[5,6]:

Exponential model

\[ \alpha'(\omega) = b_0 + b_1 \exp(-b_2 \omega) \]  

(3)
Polynomial model

\[ \alpha' (\omega) = a_0 + a_1 \omega + a_2 \omega^2 + \cdots + a_m \omega^m \]  \hspace{1cm} (4)

Here \( m \) is an integer. Figure 4 shows the baseline fitting where \( m=4 \) in polynomial model. Then the spectra with removing baselines are depicted in figure 5.

### 3.4. Peaks fitting

Each substance has its inherent peaks of spectra. And the peaks are generally overlapped or disturbed by noises. We try to recovery them by peak fitting of a Gaussian or Lorentzian function.

![Figure 6. Peak fitting](image)

In figure 6, \( T(x_0, y_0, f) \) is a peak of transmittance spectrum on pixel \((x_0, y_0)\). Make a top mark \( C \) and a cross mark \( AB \) where the amplitude is as low as possible without other peaks overlap. Then, the height \( T_c \), the intersection points \( (f_a, T_a) \), \( (f_b, T_b) \) and the width \( AB \) are calculated by the software.

Hence, the Gaussian model is

\[ T = T_0 + \frac{D}{w\sqrt{\pi}} e^{-\frac{(f-f_c)^2}{w^2}} \]  \hspace{1cm} (5)

and the Lorentzian model is

\[ T = T_0 + \frac{D}{2\pi (f-f_c)^2 + w^2} \]  \hspace{1cm} (6)
Where $T_0$ is the baseline, $w$ is the width of peak, $D$ is the area under the peak, and $f_c = (f_a + f_b)/2$ is a symmetric axis. The value of $D$ is derived from two points at different frequencies, $(f_a, (T_a + T_b)/2)$ and $(f_b, (T_a + T_b)/2, T_c)$. After all, $w$ and $D$ in Gaussian model are as following.

$$w = (f_a - f_c)[-0.5 \lg((T_a - T_0)/(T_c - T_0))]^{0.5}$$  \hspace{1cm} (7)$$

$$D = (T_c - T_0)w\sqrt{\pi}/2$$  \hspace{1cm} (8)$$

And in Lorentzian model, they are as following.

$$w = 2(f_a - f_c)[(T_a - T_0)/(T_c - T_a)]^{0.5}$$  \hspace{1cm} (9)$$

$$D = (T_c - T_0)w\pi/2$$  \hspace{1cm} (10)$$

In figure 7, the peaks fit with Gaussian and Lorentzian models are correspondingly depicted on red and green curves.

4. 3-D display of spectra

The spectrum process for a single pixel is represented above. One by one, huge mount of data form a series of 3-dimension images.

4.1. 3-D display of absorption and transmittance spectra

Figures 8 (a) and (b) represent the transmittance and absorbance spectra at specific frequency 1.1577 THz. The spectrum amplitudes and concentrations of substances are colorized according to a colour scale at the right corner.

By changing frequencies and identifying their peaks, substances included in the sample could be confirmed qualitatively. The 3-D images are shown in figure 9 at a series of frequencies.

4.2. Some considerations

In figure 8, some substances out of our interesting are completely transparent in THz scope. Extremely big transmittance would take place on those pixels, and corresponding spectra go beyond the regular range. We take them to be noises and wipe them off by an adaptive threshold.

In order to process massive data in format of NetCDF (Network Common Data Form), some tricks must be taken in case of overflow of memories and to ensure that all tasks implement in an acceptable period of time. These tricks include multiplex of variables, dynamic relocation of memories, and recall of temporal results.

![3-D display of spectra](image)
Figure 8. Reconstructed THz images at 1.1577 THz. (a) transmittance (b) absorbance

Figure 9. Reconstructed 3D THz images of transmittance at 1.1577 THz

5. Conclusion
The primary distribution of THz experiment data can be transferred to absorbance or transmittance spectra in this software. Due to be able to treat echoes, noises, baselines and peaks, it becomes powerful to qualitative and quantitative analyses of solid-state samples.

Acknowledgments
This work was supported by the National Nature Science Foundation of China (No60977065).

References
[1] X.-C. Zhang 2002 Physics in Medicine and Biology 47 3667
[2] Peter Uhd Jepsen and Bernd M Fischer 2005 Optics Letters 30 29-31
[3] Zhaohui Zhang, Zuxing Zhang, Yixin Yin, Yuko Ueno, Rakchanok Rungsawang and Katsuhiro Ajito 2009 Frontiers of Optoelectronics in China 2 239-243
[4] Taday PF, Bradley IV and Arnone DD 2003 Journal of Biological Physics 29 109-115
[5] Zhaohui Zhang, Luodong Lv, Yixin Yin, Yuko Ueno, Rakchanok Rungsawang and Katsuhiro Ajito 2007 Journal of Analytical Science 23 651-654 (in Chinese)
[6] Yamamoto K, Kabir M H and Tominaga K J 2005 Opt. Soc. Am. B 22 2417-26.