Study on Terahertz Time-domain Spectral Signatures of Wheat from Different Years

Yin Shen1,2, Li Bin2, Chunjiang Zhao1,2*, Guanglin Li1*

1 College of Engineering and Technology, Southwest University, Chongqing 400715, China
2 National Engineering Research Center for Information Technology in Agriculture, Beijing 100097, China
*Corresponding author email: zhaocj@nercita.org.cn

Abstract. Wheat freshness is an important factor affecting wheat quality. In the current research, a total of 375 wheat samples from five different years (2016, 2017, 2018, 2019 and 2020) were identified by using the terahertz time-domain spectroscopy (THz-TDS) technology. The THz spectrum information of wheat was acquired, and the THz-TDS signals of wheat were obtained after Savitzky-Golay pretreatment. Then the data of frequency-domain spectra, refractive index spectra and absorption spectra of wheat within the range of 0.2~1.4 THz were obtained after calculating the optical parameters. According to the experiment results, there were differences in the refractive indexes and absorption coefficients of wheat samples from different years. The refractive indexes of wheat samples from 2020 were significantly lower than that of wheat samples from other years, and the absorption coefficients of all five kinds of samples increased as the frequency increased. The study results showed that THz-TDS was of great potential for the effective determination of wheat freshness and it provided a basis for determination of wheat quality, bearing great practical significance.

1. Introduction

Wheat is a living plant with different physiological and biochemical properties. As the storage period extends, the organic chemicals in wheat would change as its nutrients lose, resulting in quality deterioration and finally leading to decrease in edibility. Many unscrupulous businesses mix new and old wheat for profits, causing loss to consumers. In order to ensure wheat quality, reduce economic loss and improve storage safety, it is necessary to distinguish new and old wheat, i.e. identifying wheat from different years.

The existing methods for identification of the grain freshness are mainly based on the changes of enzyme activities and chemical components in wheat. Common methods include sensory evaluation, guaiacol method, fatty acid method and tetrazolium salt staining. Although these methods can determine the grain freshness, they are not widely used in practical work due to long determination cycle, limited technical conditions and insufficient personnel capability. Therefore, the identification of wheat freshness has always been a technical issue for researchers and grain industry participants. In order to ensure the storage of quality fresh wheat, the study on methods for determining wheat freshness is of great significance.

The Terahertz (THz) wave is an electromagnetic radiation wave within the transition region of infrared wave and microwave. From the perspective of energy, the magnitude of e THz energy (about 4 meV) is between the range of those of electron and photon in the transition region from the electron...
domain to the photon domain. The THz wave features strong capacity in absorption of and resonance with most biological macromolecules, making it extensively applied in such fields as food quality determination [1], biomedicine [2], agricultural engineering[3], and mix determination [4]. Bin Li et al. [5] determined common agricultural diseases with the THz technology. Hong-yi, GE et al. [6] studied the THz spectral signatures of mildewed, insect-eaten and germinated wheat by using THz-TDS, and found that the optical parameters of such wheat were significantly different from those of normal wheat, indicating that THz-TDS could be used for identification of wheat quality. Yu-Ying, JIANG et al. [7] applied the THz imaging technology and chemometrics to determining the maltose content of wheat, and made quantitative analysis of maltose, which delivered effective determination results. Baek, S. H [8] applied the THz imaging technology to determining the presence of melamine in food, and the results showed that THz imaging can be used for the qualitative determination of melamine in food. Hong-Yi, GE et al. [9] tested the wheat samples stored in four different years, providing a new method for determining wheat freshness.

Considering the merits of THz-TDS in determination in the field agricultural engineering, THz-TDS was used to determine and identify wheat from different years based on the aforesaid studies. The time-domain spectra of wheat from different years were acquired before the absorption coefficient and refractive index spectra of the samples were obtained through calculating the optical parameters. Finally, the differences of spectra were analyzed and compared for fast identification of wheat freshness.

2. Materials and Methods

2.1 Samples
As the wheat is usually warehoused and stored for five years, the wheat samples from 2016, 2017, 2018, 2019 and 2020 were selected for the experiment. Samples were all provided by Beijing Hybrid Wheat Engineering and Technology Research Center of Beijing Academy of Agriculture and Forestry Sciences. A total of 375 properly bagged, packaged and labeled samples were obtained, comprising 75 samples from each year.

2.2 Test Instruments
The THz experiment was performed under the room temperature of 292K. During measurement, it was required to fill nitrogen inside the instrument enclosure to control the humidity inside the enclosure to below 4%, so as to reduce the influence of moisture in the air on the measurement results. Since the polyethylene did not absorb the THz wave, the polyethylene tablet was scanned with no sample placed, and the obtained polyethylene time-domain waveform signal was used as the reference signal. The sample was then placed on the sample holder for scanning, and the obtained time-domain waveform signal contained the optical information of the sample in this band.

2.3 Spectral Data Acquisition and Pretreatment
The raw data acquired by THz-TDS is the time-domain spectral data of 0~80 ps. The time-domain spectral data are often saved in TXT. The THz spectral data were acquired 3 times for each sample. In order to obtain the time-domain spectra, the refractive index spectra and the absorption coefficient spectra of the sample, the THz signal measured without any sample was used as the reference signal. Then the original time-domain spectrum signal experienced Fourier Transform to obtain the frequency domain spectrum signal, and then the refractive index and the absorption coefficient were calculated based on the thickness of each sample.

The obtained raw spectral data contained invalid interference information. In order to obtain effective spectral information, it was necessary to use appropriate pretreatment methods to eliminate the interference information, which can highlight the useful information and reduce model complexity. The common spectrum pretreatment methods for removing the interference information include mean centering, standardization, normalization, Savitsky-Golay (SG) method, derivative method, and standard normalized variate (SNV), multiplicative scatter correction (MSC), baseline correction, etc.
Among many pretreatment methods, the polynomial 15-point smoothing method was finally selected after comparison and analysis for Savitzky-Golay of the absorption spectral curve according to the experimental study in combination with the sample characteristics and the function of the pretreatment method.

3. Results and Analysis

3.1 Analysis of Terahertz Time-Domain and Frequency-Domain Spectra of Wheat from Different Years

The time-domain spectra of wheat samples from different years were obtained by THz-TDS under certain temperature and humidity conditions. The signal-to-noise ratio (SNR) of the THz-TDS of wheat samples was low at the first end and in the high frequency band, which contained much noise resulting in great data error. Savitzky-Golay was used to pretreat the spectral data to reduce the influence of noise, sample particle size and optical path on the spectra. After spectrum pretreatment, the THz-TD curve is shown in Fig. 1.

From Figure 1, the time-domain signals of wheat samples from different years show delay and amplitude attenuation compared with the reference signal. In the time-domain spectra, the attenuation of amplitude was due to the absorption of the sample. The time-domain spectrum signals of samples in different years had different time delays, which indicated different refractive indexes of the samples. Through the Fourier transform calculation, the frequency-domain spectra of wheat from different years were obtained, as shown in Fig. 2. From the frequency-domain spectra, the peaks at 0.48THz and 0.60THz in the reference signal may be caused by absorption of moisture contained in the air. The cut-off frequency of saturated absorption of wheat samples from different years is 1.4THz. Due to the low SNR in the range of 0 ~ 0.2THz and 1.4 ~ 2THz, the frequency in the range of 0.2 ~ 1.4THz was selected for the study. When they were compared with the reference signal, the amplitudes of different wheat samples decreased to different degrees, with the smallest amplitude in the wheat samples of 2020 and the largest amplitude in that of 2016. As the wheat samples were measured under the same experimental conditions, the differences in time-domain amplitudes indicated different absorption of THz by wheat from different years, and narrow frequency spectra of wheat samples from different years in the high frequency part, which was also caused by absorption.
3.2 Analysis of Terahertz Absorption Coefficients and Refractive Index Spectra of Wheat from Different Years

In the study, the absorption coefficient spectra and refractive index spectra of wheat samples from different years were calculated by applying the method in the references [10] based on different time-domain signals. Fig. 3 shows that the refractive indexes of wheat samples are different to some extent, with small change in refractive index curves of the wheat samples from different years. The refractive indexes change slowly in the range of 0.2~0.6THz without significant dispersion, while the refractive indexes decrease slowly in the range of 0.6~1.4THz as the frequency intensifies, which suggests small anomalous dispersion. Small change in refractive indexes is the evidence of less prominent dispersion. The signal jitter of wheat samples from different years in the range of 0.1~0.2THz is caused by the interference from the low SNR of the experimental system. In the frequency range of 0.2~1.4THz, there is a large refractive index difference between the wheat samples from 2020 and those from 2017, and the value of the refractive indexes of the wheat samples from 2020, 2019, 2018, 2017 and 2016 at 0.8THz are 1.0021, 1.0057, 1.0066, 1.0081 and 1.0073 respectively. After analysis, it is found that the refractive index curves of wheat are different due to the different years of wheat, but there is no significant dispersion. According to the Cauchy Law, no strong selective absorption characteristics would occur in the 0.2~1.4 THz absorption coefficient spectra curve, in other words, there would be no obvious characteristic absorption peak.
Fig. 4. Absorption coefficient spectra of samples.

The absorption spectral data of wheat samples are shown in Fig. 4. It can be seen from the figure that the THz absorption spectra of wheat samples from different years show no obvious absorption peak. In the range of 0.2~1.4THz, the absorption coefficients of five kinds of wheat samples increase gradually as the frequency intensifies. Among them, the absorption coefficient of wheat samples from 2020 is the highest, implying strongest absorption but without characteristic absorption. At 0.8THz, the wheat from 2020 has the largest absorption coefficient of 4.3298, and the wheat from 2017 has the lowest absorption coefficient of 2.98. Although there are no obvious absorption peaks in the absorption spectra of wheat samples from different years, wheat samples from different years can also be identified considering different absorption spectra curves of different samples.

4. Conclusion

Through the experimental study of wheat samples from five different years in the THz bands, it was found that different wheat samples had similar THz band, indicating that wheat from different years had the same main components. The refractive index spectra suggested that there were differences in refractive indexes of wheat from different years. There was no characteristic absorption peak in the absorption spectra curve, and the absorption coefficient increased as the frequency intensified. The wheat from different years can be identified according to such optical properties as absorption and refraction of wheat samples stored in different years. If the THz spectra of wheat samples from different years were basically the same, further identification was needed by using chemometrics, or as an alternative, spectral recognition algorithm can be applied to extract effective information. The study provided a reference method for the use of THz-TDS in fast determination of grain, bearing great significance for better warehousing and storage.

Acknowledgments

This research work was supported by the National Key Research and Development Project of China (2016YFD0702002).

References

[1] Ok, G.; Shin, H. J.; Lim, M.-C.; Choi, S.-W., Large-scan-area sub-terahertz imaging system for nondestructive food quality inspection. Food Control 2019, 96, 383-389.
[2] Kim, K. W.; Kim, K. S.; Kim, H.; Lee, S. H.; Park, J. H.; Han, J. H.; Seok, S. H.; Park, J.; Choi, Y. S.; Kim, Y. I., Terahertz dynamic imaging of skin drug absorption. Optics Express 20, (9), 9476.
[3] Li, B.; Yuan, L.; Liu, H.; Zhao, C., Research progress on Terahertz technology and its application in
agriculture. *Transactions of the Chinese Society of Agricultural Engineering* 2018.

[4] Liu, W.; Zhang, Y.; Li, M.; Han, D.; Liu, W., Determination of invert syrup adulterated in acacia honey by terahertz spectroscopy with different spectral features. *Journal of the Ence of Food and Agriculture* 2020, 100, (5), 1913-1921.

[5] Li, B.; Zhang, D.; Shen, Y., Study on terahertz spectrum analysis and recognition modeling of common agricultural diseases. *Spectrochimica Acta. Part A, Molecular and Biomolecular Spectroscopy* 2020, 243, 118820-118820.

[6] Ge, H.; Jiang, Y.; Xu, Z.; Lian, F.; Xia, S., Identification of wheat quality using THz spectrum. *Optics Express* 2014, 22, (10), 12533-12544.

[7] Jiang, Y. Y.; Ge, H. Y.; Zhang, Y., Quantitative analysis of wheat maltose by combined terahertz spectroscopy and imaging based on Boosting ensemble learning. *Food Chemistry* 2020, 307, 8.

[8] Baek, S. H.; Lim, H. B.; Chun, H. S., Detection of Melamine in Foods Using Terahertz Time-Domain Spectroscopy. *Journal of Agricultural & Food Chemistry* 2014, 62, (24), 5403.

[9] Hong-Yi, G. E.; Yu-Ying, J.; Hai-Hua, M. A.; Fei-Yu, L.; Yuan, Z.; Shan-Hong, X., Study on Rapid Nondestructive Evaluation of the Freshness Wheat Using Terahertz Time Domain Spectroscopy. *The Journal of Light Scattering* 2015.

[10] C, Y. S. A.; B, Y. Y.; C, B. L. B.; C, C. Z. A.; A, G. L., Detection of impurities in wheat using terahertz spectral imaging and convolutional neural networks - ScienceDirect. *Computers and Electronics in Agriculture* 181.