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Terahertz Spectroscopic Study of Standard Substances for Bituminous Coal and Anthracite

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Abstract: This study underscores the significance of online monitoring of standard substances for bituminous coal and anthracite, two commonly used fossil fuels. Terahertz technology emerges as a powerful non-destructive detection method capable of revealing the physical and chemical properties of measured objects. In this research, terahertz time-domain spectroscopy technology was employed to investigate the spectral characteristics of four distinct types of bituminous coal and anthracite samples. The refractive index and absorption coefficient spectra of these samples were calculated across a frequency range of 0.5 THz to 2.5 THz. Furthermore, principal component analysis was conducted using all refractive index and absorption coefficient data within this frequency band. Through the analysis and comparison with known parameters of coal standard materials, it was established that carbon content primarily influences the refractive index of bituminous coal and anthracite, while ash content predominantly affects the absorption effect. These findings underscore the potential of terahertz spectroscopy in conjunction with principal component analysis to qualitatively assess the similarities and differences between coal samples, thus offering novel insights for the online monitoring of diverse coal types and qualities.

Keywords: Coal; Terahertz spectroscopy; Optical parameters; Principal component analysis

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1. Introduction

China has abundant coal resources, and as a major producer and consumer of coal in the world, coal plays an important strategic role in the development of China's national economy [1,2]. Coal can be divided into three types according to the degree of coalification: brown coal, bituminous coal, and anthracite. The prices and uses of different coal types vary, and so do the environmental pollution they cause. To achieve carbon neutrality [3-4], there is an urgent need to develop methods for quickly and accurately monitoring key parameters and elements in coal online.

Bituminous coal and anthracite consist of both organic and inorganic matter. The main elements of organic matter include carbon, nitrogen, oxygen, hydrogen, and sulfur. The composition of the elements can be detected through laboratory analyses. In industrial production, online monitoring technology plays a crucial role in quickly assessing coal quality. Over recent years, terahertz technology has gained significant traction, showing promising applications in non-destructive testing [5-8] and drug identification [9-11]. Wang *et al.* differences in the responses of various coal types within the terahertz frequency band, with several coal components impacting the terahertz constant [12-15]. Building upon these findings, this article utilizes a machine learning algorithm known as principal component analysis to analyze the refractive index and absorption coefficient data obtained from terahertz measurements. By correlating these processed results with the primary physical properties of bituminous coal and anthracite, the study aims to investigate the influence of different coal components on terahertz optical parameters.

2. Experiments and methods

The experiment utilized the TAS 7400SU transmission THz-TDS system from Advantest, Japan, for detecting coal samples. To minimize experimental errors, the air humidity in the optical path was maintained below 1% RH, and sample data was measured at a temperature of 24°C. Each sample was subjected to three repeated measurements, and the average value was taken as the sample information. Two types of coal powder were employed in the experiment: anthracite (ZBM097A) and bituminous coal (ZBM102, ZBM111A, ZBM111C). **Table 1** presents the chemical composition and physical properties of the four coal samples.

Table 1. Encoding and property parameters of four coal samples

Content (%)	Coal number			
	ZBM097A	ZBM102	ZBM111A	ZBM111C
Carbon	79.96	57.82	74.16	77.14
Hydrogen	3.31	3.40	4.44	4.59
Nitrogen	1.12	1.02	1.38	1.26
Volatile	8.99	30.43	33.64	31.29
Ash	11.87	25.88	9.62	8.00

3. Results and discussion

3.1. Terahertz spectroscopic analysis

After performing Fast Fourier Transform (FFT) on the terahertz spectrum containing physical information of the tested sample, the refractive index spectrum and absorption coefficient spectrum of the sample were calculated using optical parameter calculation formulas [16-18]. **Figure 1 (a)** displays the refractive index spectra of four coal samples in the 0.5-2.5 THz band. Significant differences in the refractive index spectra of the four coal samples in the terahertz band were evident. Anthracite ZBM097A exhibited the highest refractive index spectrum, with an average refractive index of 1.60, notably higher than that of bituminous coal. Therefore, terahertz technology could be utilized for the initial calibration of anthracite in rapid coal identification. The average refractive index spectra of ZBM111C, ZBM111A, and ZBM102 bituminous coal decreased sequentially, with values of 1.54, 1.52, and 1.47, respectively, all lower than those of anthracite. Additionally, the refractive index of ZBM102 coal demonstrated a clear trend of initially increasing and then stabilizing. The average refractive index of all samples was plotted against the carbon content of the samples, revealing the relationship between the carbon content in the samples and the average refractive index spectrum (K), as depicted in **Figure 1 (b)**. According to the data fitting, the average refractive index increased exponentially with carbon content.

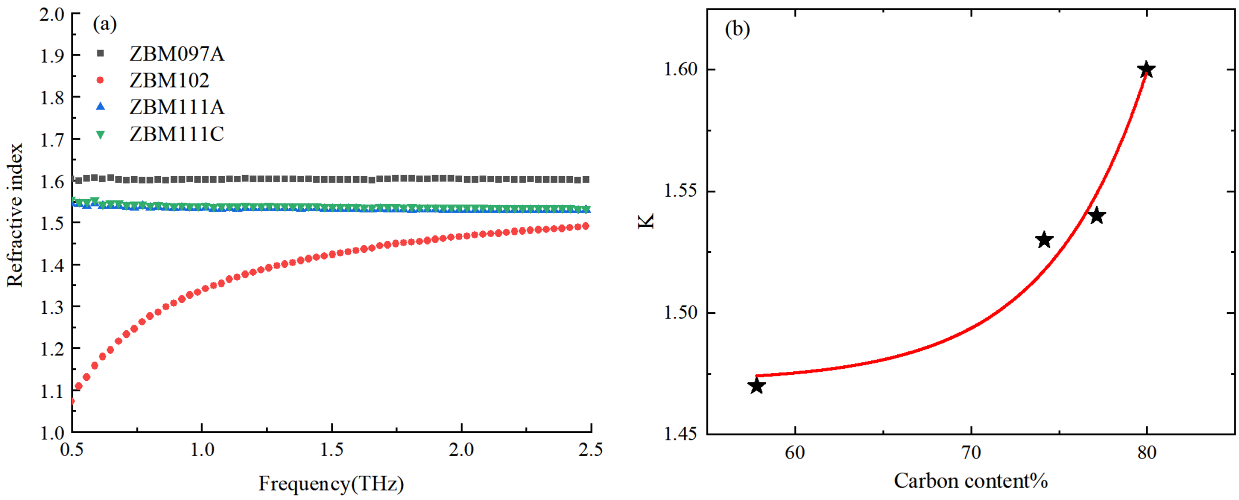

Figure 1. (a) Terahertz refractive index spectra of each sample, (b) relationship between carbon

Figure 2(a) displayed the absorption coefficient spectra of four samples within the frequency range of 0.5–2.5 THz. The absorption coefficients of the four samples increased with the frequency, and within the specified frequency range, the overlapping positions of absorption peaks resulted in no distinctive characteristic absorption peak in the absorption coefficient spectrum. The relative order of absorption coefficients of the four samples at various terahertz frequencies remained consistent, with ZBM111C exhibiting the smallest absorption coefficient and ZBM102 displaying the largest absorption coefficient. Through data fitting, it was determined that the absorption coefficient slopes of the four samples were 18.72, 18.88, 16.31, and 12.26, respectively. Plotting the slope of the absorption coefficient of each sample against the ash content of the sample revealed the relationship between the change in ash content in the sample and its absorption coefficient change, as depicted in **Figure 2 (b)**. From **Figure 2 (b)**, it was observed that there was an approximately identical trend between the ash content of the sample and the slope of the absorption coefficient (S).

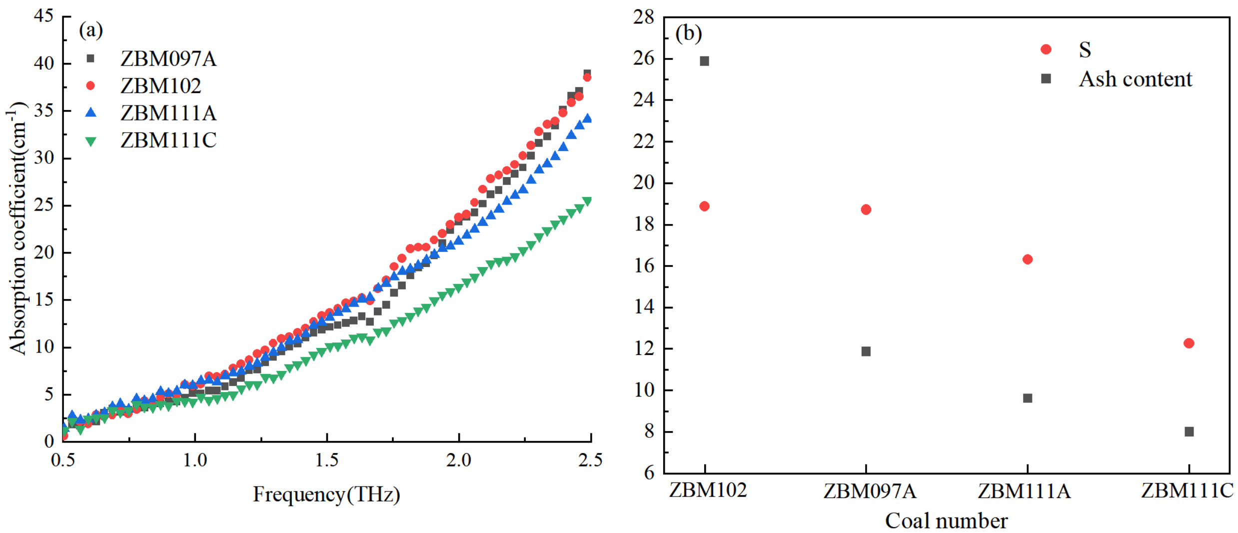

Figure 2. (a) Terahertz absorption coefficient spectra of each sample, (b) variation of ash content and absorption spectrum slope (S) in the samples

3.2. Principal component analysis

Principal Component Analysis (PCA) is a statistical technique that converts a set of correlated variables into a set of linearly uncorrelated variables through orthogonal transformation [19-20]. hese transformed variables are termed principal components. Each principal component encapsulates unique information, with the first principal component containing the highest amount of information. By examining the scores of the first principal component, one can discern the interrelationships between samples, facilitating sample classification.

Figure 3(a) displays the two-dimensional principal dispersion point plots of each sample obtained by using the refractive index spectrum as the input variable. The scatter plot revealed a significant clustering effect of the four samples on PC1, wherein the closer the distance between samples, the higher the similarity; conversely, the farther the distance, the greater the difference. Among them, sample ZBM111A was closest to ZBM111C, followed by ZBM097A. ZBM102 was distant from the other three samples and had the smallest PC1 score, markedly differing from the others. By comparing the PCA results with the known physical properties of the samples, it was concluded that carbon content was the main factor affecting the refractive index of coal materials in the terahertz band. The carbon content of ZBM111A and ZBM111C was 74.16% and 77.14%, respectively, with a relatively small difference. In contrast, the carbon content of ZBM102 was 57.82%, significantly differing from the other samples. Corresponding to **Figure 3 (a)**, ZBM102 appeared farthest from the other samples. Therefore, there was a certain correspondence between the relative values of carbon content and the differences in refractive index among the samples. Additionally, other parameters such as ash content also affected the refractive index of coal in the terahertz frequency band to varying degrees. As the ash content increased, the average refractive index of the sample decreased relatively. This demonstrates that their similar refractive indices result from the combined effect of various physical parameters. Consequently, the refractive index of coal in the terahertz frequency band is determined by a combination of all physical properties, with carbon content being the most influential factor.

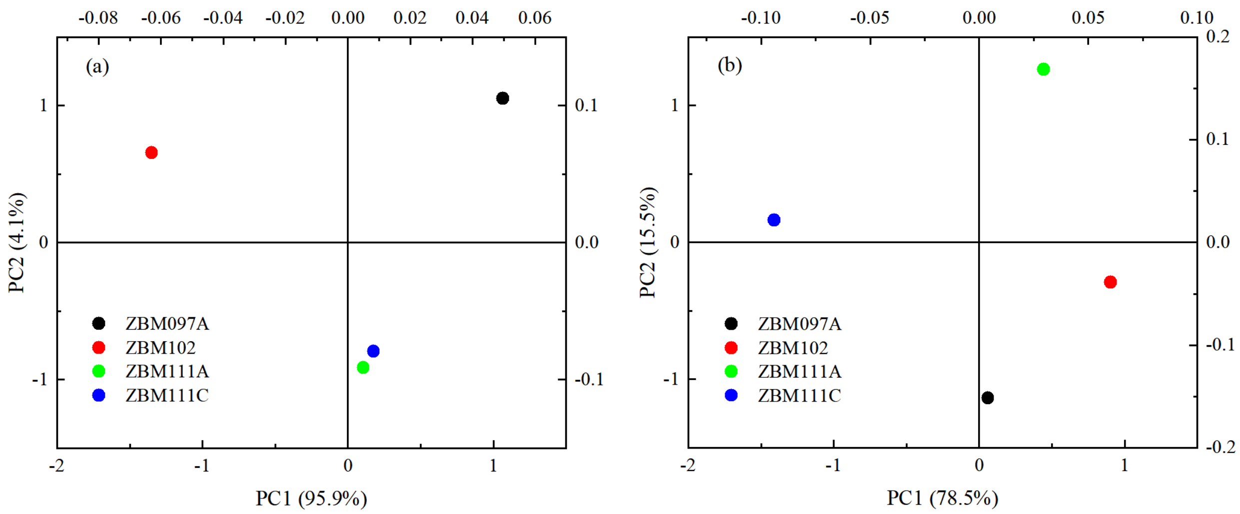

Figure 3. (a) Two-dimensional principal dispersion point plots of the sample based on refractive index spectrum, (b) two-dimensional principal dispersion point plots of the sample based on absorption coefficient spectrum.

Similar to the above analysis process, all absorption data in the frequency range of 0.5 THz to 2.5 THz were utilized as input variables to compute a two-dimensional principal component dispersion point map based on the absorption coefficient spectrum, as depicted in **Figure 3 (b)**. From the graph, it could be observed that the positions of the four samples were relatively independent. ZBM111C exhibited the lowest PC1 score, followed by an increase in PC1 scores for ZBM111A, ZBM097A, and ZBM102. Among the main components of the sample, the ash content showed the same trend of change as the PC1 score. Therefore, the ash content was the primary factor affecting the absorption coefficient of coal substances in the terahertz band. Meanwhile, the content of volatile matter in the sample mirrored the PC2 score pattern: ZBM097A had the lowest volatile matter content, corresponding to the lowest PC2 score of ZBM097A. The difference in volatile content among the other three samples was relatively small, and the corresponding PC2 scores of the three samples in the figure were similar. Hence, the absorption coefficient of coal in the terahertz frequency band was also determined by a combination of all physical properties, among which ash content was the most influential factor.

4. Conclusion

Terahertz spectral tests were conducted on four bituminous coal and anthracite samples, and their refractive index spectra and absorption coefficient spectra were calculated. The findings revealed significant variations in terahertz optical parameter spectra among coals with different component contents. Principal component analysis was conducted on the data to delve deeper into the refractive index and absorption coefficient of the samples in the terahertz band. It was found that each component influences the coal's refractive and absorption coefficients to varying degrees, with carbon content primarily affecting the refractive index and ash content primarily impacting the absorption coefficient. The analysis effectively discerned similarities and differences between coal samples. By expanding the dataset to include more coal types, machine learning methods could be utilized to further analyze terahertz optical parameters, aiding real-time online monitoring of coal quality and types.

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Disclosure statement

The authors declare no conflict of interest.

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