Analysis on Scattering and Relationship with granular size in THz spectra

Fang M. Wu[1], Bing F. Wu[1], Xiao Y. Zhao[2*], Zhao H. Zhang[2], Han. Zhang, Tian Y. Zhang[2] ,Yan. Fang[2]
[1]Key Laboratory of Digital Earth Sciences, Institute of Remote Sensing and Digital Earth, Chinese Academy of Sciences, Beijing 100101, China
[2]Department of Instrumentation Science, University of Science & Technology Beijing, Beijing 100083, China

***Abstract*—Scattering is an important phenomenon and distorts the THz absorption spectrum during analysis of materials. It is essential to understand how scattering from samples changes the THz signals. We presented an approach for estimating the relationship between scattering and granular sizes occurring in THz spectra. The samples were made of same solid material but in different granular sizes ranging from 58um to 150um. The experiment spectra indicated the absorption curves rose up with the granular size increasing, which met the simulation consequence based on Mie scattering. The empirical baseline models were presented in this paper, after removing the baseline, the result indicated that computational accuracy was improved, which can be used in quantitative analysis.**

I. INTRODUCTION

Frequency dependent absorption of a given material at distinct frequencies in the terahertz (THz) range has been successfully used as a spectral fingerprint in the qualitative analysis of materials. However, the quantitative results are of great error due to these fingerprint features being distorted by the sample's scattering to the THz ray.

THz radiation scatters from sample particles, which leads to an obvious baseline increasing with frequencies in absorption spectrum. There are various factors involved in scattering, firstly the relationship of granular size and scattering was studied in this paper. By concluding the influences of granularity factors to the scattering, the granular coefficient in the scattering model will be determined and validated by experiments, it is a key point of eliminating scattering and benefit to the accuracy of the THz spectrum analysis.

II. EXPERIMENTS

Sucrose (refined sugar) and salt were selected as the experiment materials, which can be easily ground into different sizes. They are the ideal and cheap materials to study scattering, we control the granular size with standard sieves. With the certain diameter salt being mixed with polyethylene (PE), the powder was compressed into pellet under 8MPa. The thicknesses of samples mechanically determined are about 1 mm. The PE (from Sigma-Aldrich co. Ltd) is in form of 50μm granules without further grinding.

TABLE I Sample list

Item	Sample name	Sample name	Particle diameter(um)
1	Sugar1	Salt1	80um<d<=150um
2	Sugar2	Salt2	75um<d<=80um
3	Sugar3	Salt3	58um<d<=65um
4	Sugar4	Salt4	d<=58um

All samples were tested by the transmission THz-TDS at room temperature (23 ℃), humidity less than 3 %.The absorption spectra were shown in Fig.1.

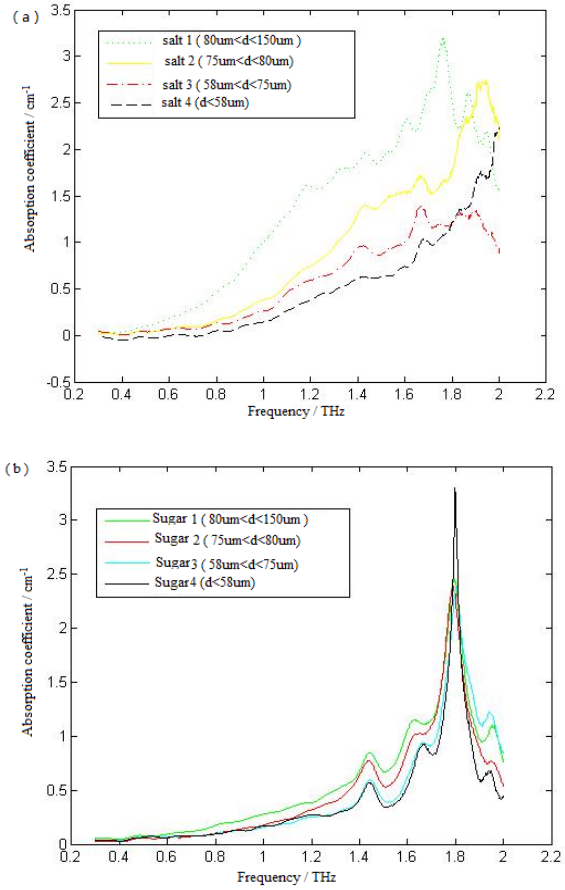

Fig. 1. Absorption spectra of different granular sizes ranging from 58um to 150um. (a) the samples are made from salt; (b) the samples are made from sugar; In each figure, four samples possess the similar absorption curves, while the absorption coefficients rise up apparently with the granular sizes ranging from 58um to 150um (0.3-2THz).

We believed that the THz radiation scatters by sample particles, which lead to an apparent baseline increasing with frequencies. The baseline affected the measurement accuracy due to additional height of spectrum. A scattering model could be set up with the experiment data, which include the information of the granular size and scattering.

III. RESULT AND DISCUSSION

Firstly terahertz absorption spectrum of samples were obtained by the terahertz time-domain spectroscopy, the relationship between different granular sizes and their absorption spectrum was analyzed, the absorption characteristic. The study finds that scattering baseline of the sample has a close relationship with the particle size.

Secondly, Rayleigh scattering theory was used in the case that particle size is smaller than the wavelength of the incident

ray, while Mie scattering theory was used in the case that particle size is close to or greater than the wavelength of the incident ray, however, but the granular size over 95 um does not follow the Mie scattering theory.

In order to remove the baseline caused by scattering, we built a model to describe the relationship between particle size and scattering in the terahertz absorption spectrum.

As we know the relationship between scattering intensity and wavelength with Mie scattering, as (1)

$$I \propto 1/\lambda^n \quad (1)$$

Here: I is the scattering intensity, λ is the wavelength, n is related with the granular size shifting from 1 to three.

After thousands of calculation, we got the empirical baseline model with our experiment data, as (2), (3).

$$I_{sugar} = 2.908*10^{-5} * f^3 * d^2 \quad (2)$$

$$I_{salt} = 3.489*10^{-5} * f^3 * d^2 - 0.05 \quad (3)$$

Here: f is the terahertz frequency, d is the granular diameter.

We believed the different coefficients in (2) and (3) are related with the material density.

The absorption spectra are shown in Fig.2. The samples in smaller granular size are almost coincident, the sugar samples fit even better. The sample salt1 with greater particle size over 80um showed greater deviation.

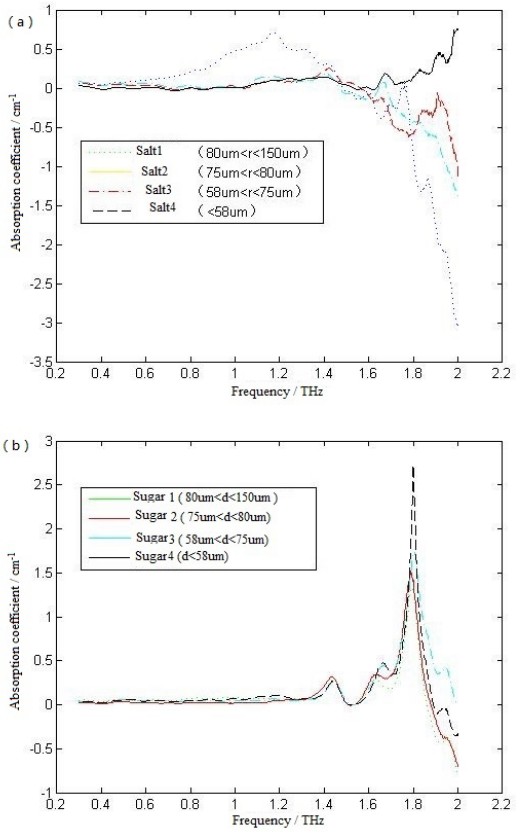

Fig. 2. Absorption spectra after removing the baseline. (a) the samples are made from salt; (b) the samples are made from sugar; four samples possess the similar absorption curves almost coincide, especially in the sugar samples.

From the Fig 2. (b), we can find the sugar has three fingerprint peaks at 1.43THz、1.65THz、1.80THz respectively. After removing the baseline and normalization in mass, the sugar samples in different concentrations are with same consistency. We selected the absorption coefficients of four samples in the 1.43 THz, with the prior samples concentration data, the normalization mass absorption coefficients (A/C) can be achieved in table II.

Except the sugar 2 has the A/C in 1.305, the other three samples' A/C about 1.18-1.21, the relative errors are in 3%. We thought that the greater error in sugar 2 may be caused from experiment, but the empirical baselines in salt and sugar were practical.

TABLE II Normalization of different samples after removing scattering baseline

Item	Sample name	Absorption coefficient (A)	Concentration(C)	A/C
1	Sugar1	0.2726	0.2276	1.198
2	Sugar2	0.2977	0.228	1.305
3	Sugar3	0.2669	0.2244	1.189
4	Sugar4	0.2713	0.2253	1.204

Comparing salt and sugar THz absorption spectra based on the current scattering models, the result indicated that the empirical baseline model can improve the computational accuracy, which can be used in quantitative analysis. Further model will be studied in improving and validating the scattering models with size information to fit and remove the scattering baseline accurately. It is an important role to optimize the terahertz system and promote the terahertz's application in qualitative and quantitative analyses.

IV. SUMMARY

The scattering is related with the granular sizes, the larger the particle the higher scattering baseline. During the sample preparation, we can control the granular in a proper size to reduce the scattering influence in THz experiment. After removing the baseline with the empirical models, the result indicated that computational accuracy was improved, which can improve the THz spectra analysis accuracy.

ACKNOLEDGEMENT

The work was supported by the National Nature Science Foundation of China (61302007) and National Science and Technology support program (2013BAD17B05). .

REFERENCES

[1]. M. Kaushik, B.W.-H. Ng, B. M. Fischer and D. Abbott, "Terahertz scattering by granular composite materials: An effective medium theory," *Applied Physics Letters,* vol. 100, pp. 011107, 1, 2012.

[2]. M. Franz, B.M. Fischer, and M. Walther, "The Christiansen effect in terahertz time-domain spectra of coarse-grained powders," *Applied physics letters*, Dove Press, vol. 92, pp. 021107, 2008.

[3]. G. M Png, C. Fumeaux, M.R Stringer, R. E Miles and D. Abbott, "Terahertz scattering by sub wavelength cylindrical arrays," *Optics Express*, vol. 19, pp. 10138-10152, 2011.

[4].B. Sengupta, Barat R, et al. "Effects of scattering on THz spectra of granular solids," *International Journal of Infrared and Millimeter Waves,* vol. 28, pp. 969-978, 2007.

[5]Z. L M, O. B, W. D P, et al. "Terahertz scattering from granular material," *JOSA* B, vol. 24, pp. 2238-2243, 2007.