Study of Scattering Distribution for Spherical Particles

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Contents

Introduction

- Terahertz (THz) waves are also known as sub-millimeter waves or T-rays.
- THz region is located in between the mid-infrared and microwave region of the electromagnetic (EM) spectrum.
- It bridges the gap between the classical to the quantum region of EM spectrum.

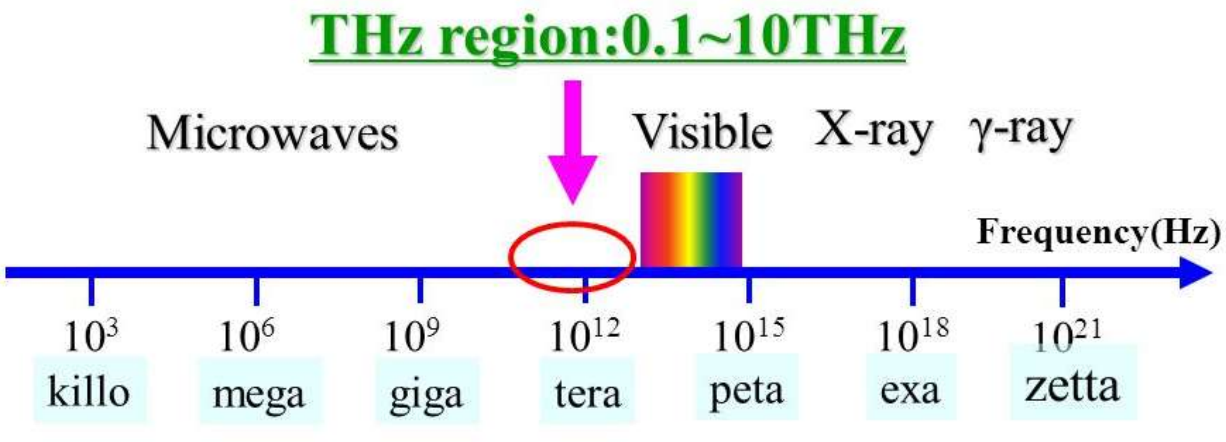


Figure 1. Location of THz region in Electromagnetic spectrum.

http://slideplayer.com/slide/8213862/25/images/3/What+is+a+THz+wave+THz+region:0.1~10THz+300%C2%B5m+%E3%83%BBWavenumber+33cm-1.jpg

- Frequency: 0.1 THz – 10 THz
- Wavelength: 3000 µm - 30 µm
- Wavenumber: 3.33564 cm^{-1} - 333.56413 cm^{-1}
- Energy: 0.41357 meV - 41.35668 meV

Distinct properties and applications of THz

- THz radiation cannot photoionized the sample due to its low photon energy which makes it suitable for Agri-Food and bio samples.

- THz radiation excites molecular specific vibrational and rotational transitions and leads to the fingerprinting of molecules.

- Most dielectrics are transparent in THz region, hence, detection through packaging is possible.

- THz is highly sensitive for presence of water which allows water estimation in plants.

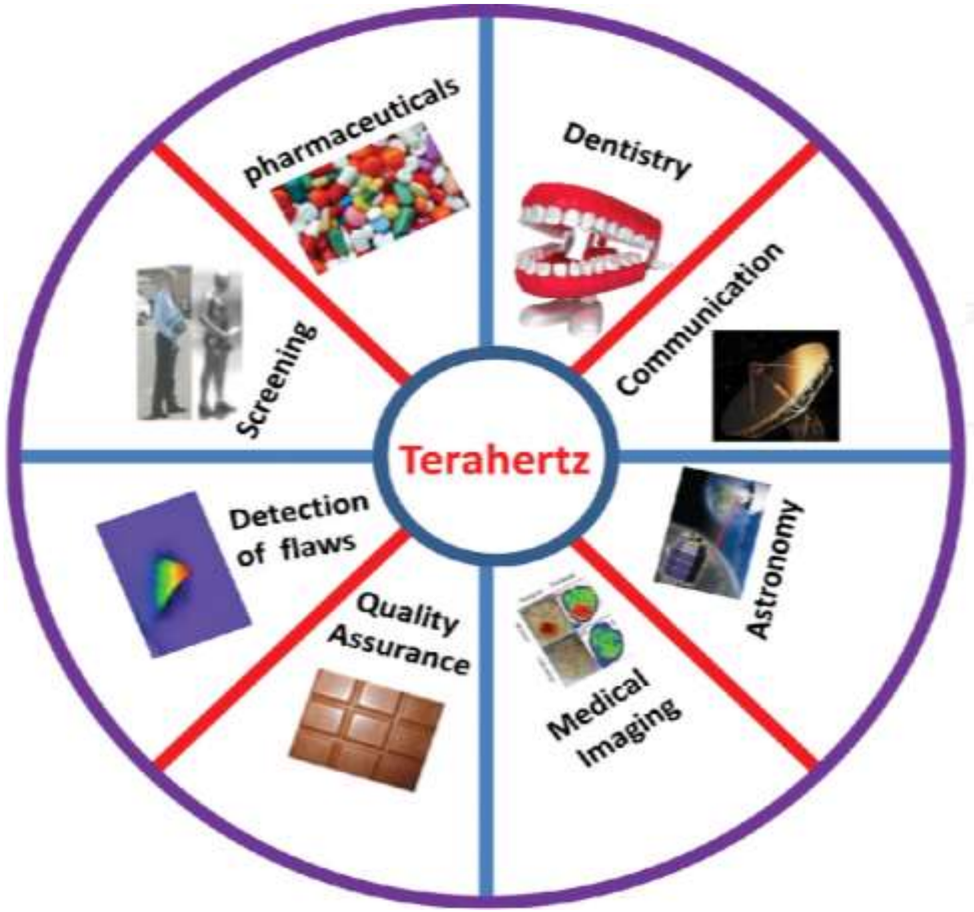


Figure 2. Applications of THz spectroscopy in various fields.

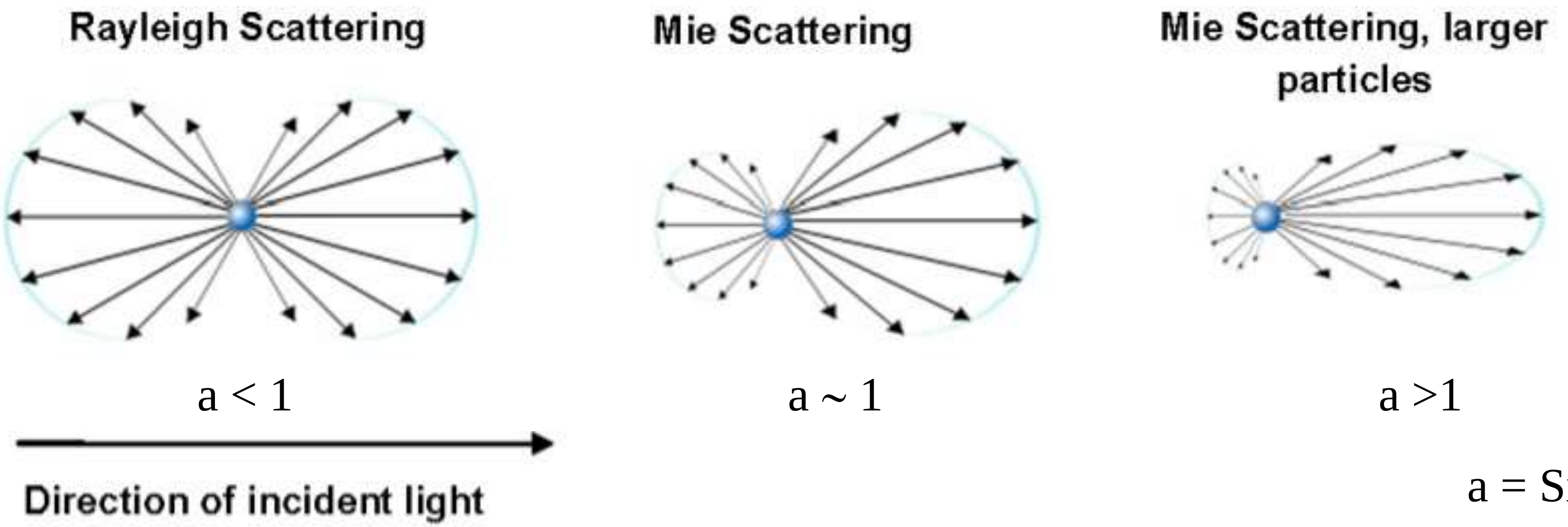
Source - https://www.semanticscholar.org/paper/Chapter-1-Terahertz-(-THz-)-Spectroscopy-%3A-A-%E2%80%90-Edge-Ghann-Uddin/a6831c9668c555c579ec8ca4d67b2bd98259fe91/figure/2

Scattering

- THz can excite molecular specific vibrational and rotational transitions. The unknown samples can be identified based on their spectral signature.

- There are some obstacles such as scattering which can influence the true spectral signature of the material and make the identification difficult.

- Scattering effect become predominant whenever the particle size of the sample is comparable to the THz wavelength (1 THz ~ 300 μm).



a = Size parameter

Figure 3. Scattering distribution with different particle size.

http://hyperphysics.phy-astr.gsu.edu/hbase/atmos/blusky.html

Proposed Model

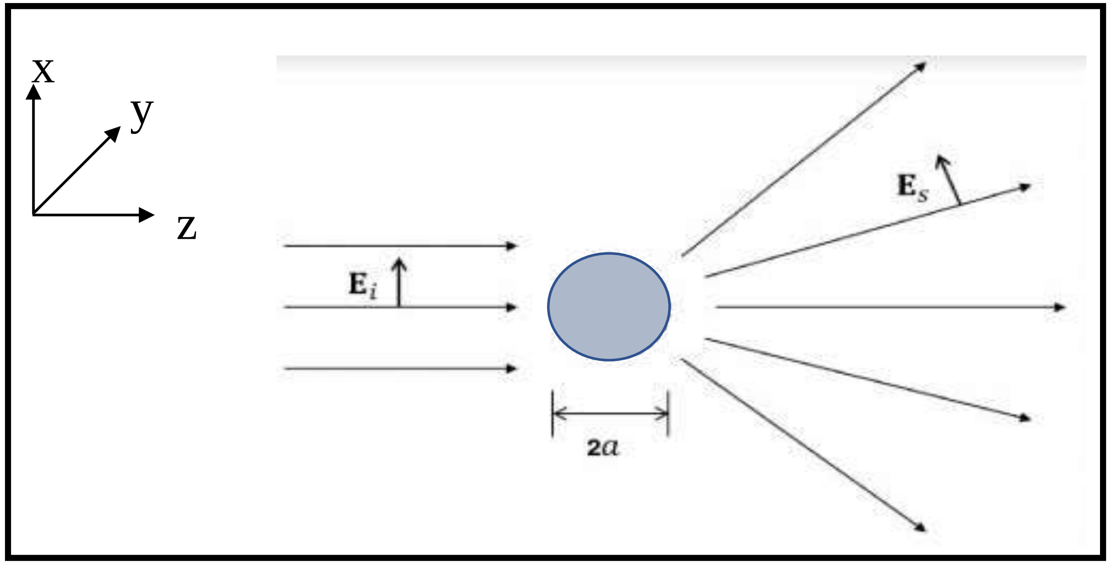


Figure 4. 2D representation of proposed model.

- Spherical Particle of different size (20 µm & 100 µm)
- Three different materials (sugar, sugar free & Teflon)
- Incident linearly polarized light (along x axis)
- Absorption coefficient obtained using THz-TDS

Scattering cross-section is a parameter used to define the scattering responses and described as the ratio of rate of energy flow of scattered radiation to the intensity of incident radiation

$$C_{sca} = \frac{W_{sca}}{I_i}$$

Here, W_{sca} is the net rate of energy flow crossing the surface of the particle, I_i is the intensity of incident radiation.

Simulation Method

Model wizard	• 3D model (spherical particle of 20 μm and 100 μm).
Module	• Proposed model simulated using Electromagnetic Waves-Frequency Domain interface available in wave optics module.
Perfectly matched layer (PML)	• PML was selected with radius ten times the radius of the particle and with thickness three times the particle radius.
Materials	• Material considered for the particles were user-defined to have variable refractive indices with frequency.
Mesh	• PML layer and particle domain were discretized using physics-controlled mesh elements.
Study	• Scattering cross-section were calculated using parametric sweep in the defined frequency range with step size 1GHz.

Result and Discussions

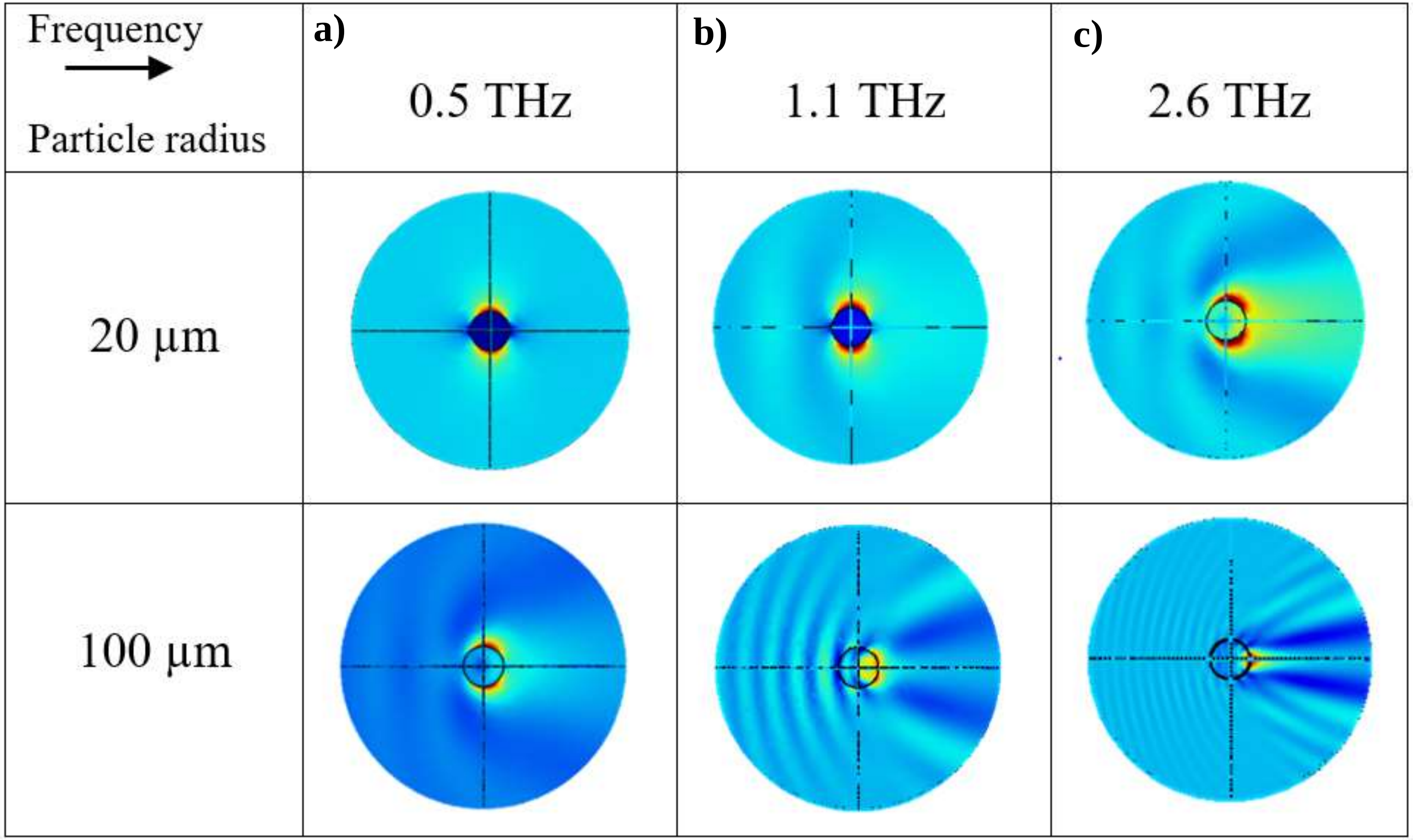


Figure 5. Scattered electric field for Teflon of 20 µm and 100 µm radius at frequencies; a) 0.5 THz, b) 1.5 THz, and c) 2.6 THz.

Result and Discussions

Figure 6. Distribution of scattered electric field for Teflon of a) 20 µm and, b) 100 µm radius at different frequencies.

- In case of 20 µm radius, the electric field retains its polarization state at low frequencies.
- As the frequency of incident radiation increases, electric field is directed towards the forward direction.
- For 100 µm radius, due to the large particle size, electric field is primarily in the forward direction even at smaller frequency (0.5 THz).
- For higher frequencies, alternative minima and maxima were observed due to the diffraction.

Results and Discussions

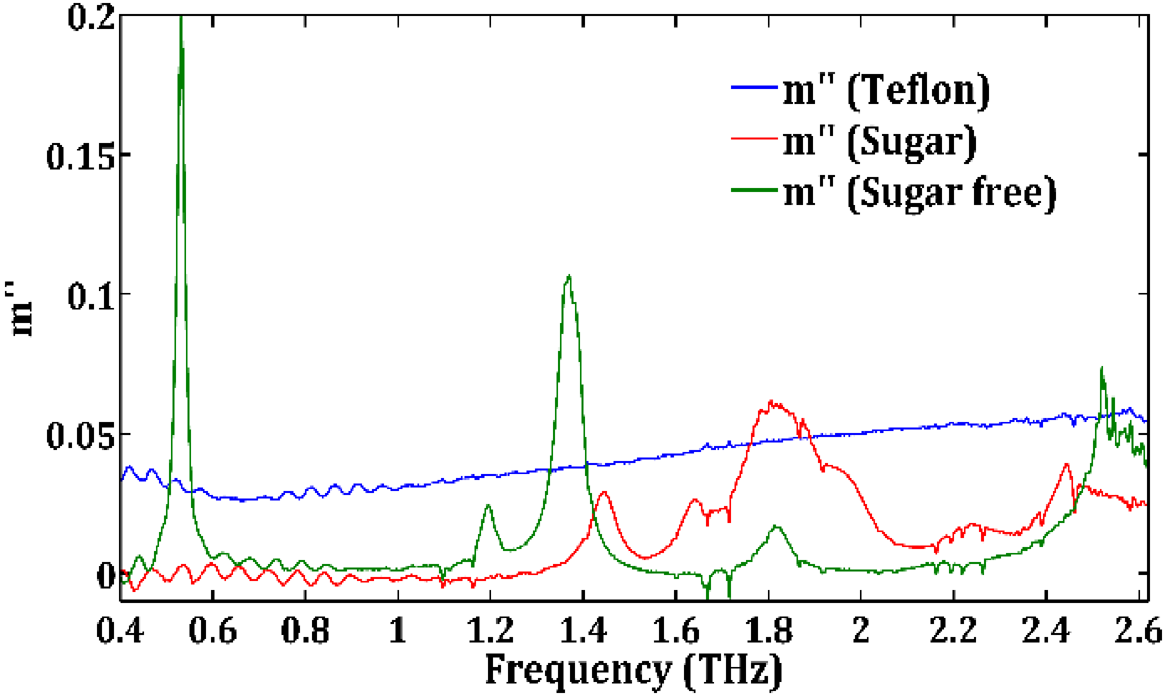


Figure 7. Plot for imaginary part of refractive index for sugar, sugar free powder, and *Teflon*.

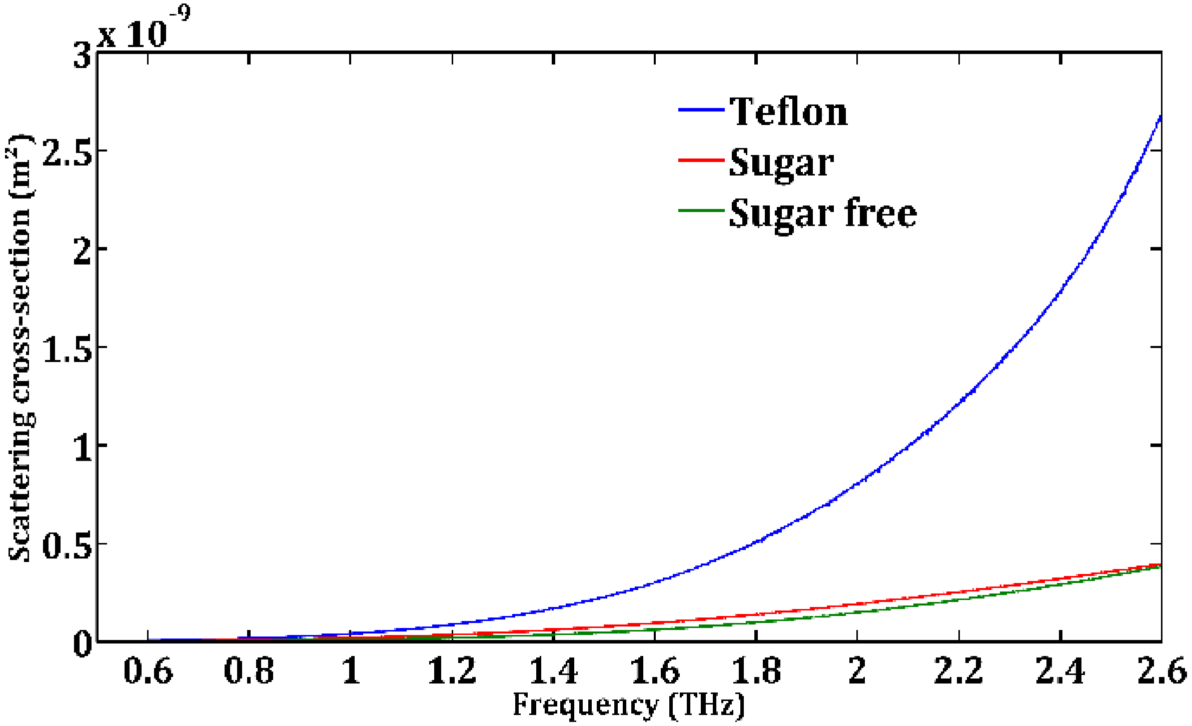


Figure 8. Scattering cross-section for 20 μm radius.

Result and Discussions

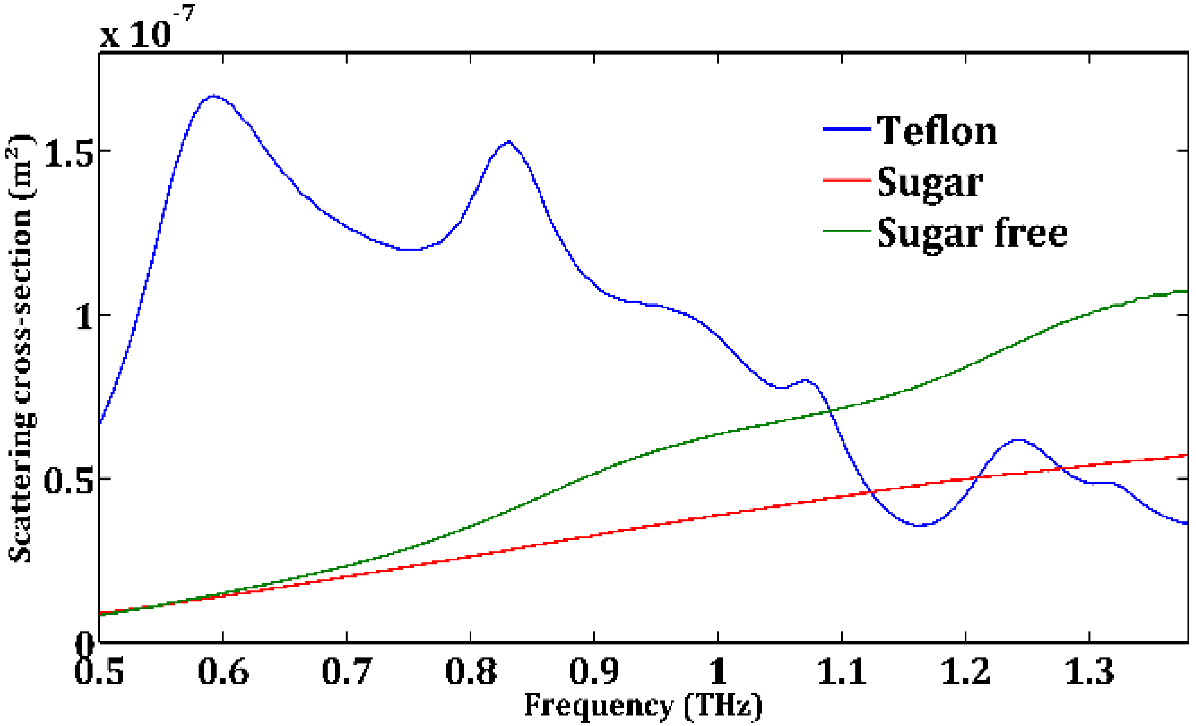


Figure 9. Plot for scattering cross-section of each particle with radius 100 µm.

- Scattering cross-section (C_{sca}) is small for initial frequency values and increases with the frequency.
- Due to the large particle size, scattering for each particle increases significantly as compared to previous case (20 µm).
- Series of board minima and maxima were obtained due to the interference of incident and forward-scattering radiation.

Conclusions and Future work

- COMSOL provides a good understanding of different optical responses for a wide range of frequency.
- Based on the COMSOL results, a frequency range can be defined for the precise study of different optical phenomenon.
- The simulated model can help to eliminate the scattering effect from the frequency spectra, and it can be extended to predict the scattering contribution from complex material for real time applications.
- In the study, it was observed that scattering response differs for absorbing and non-absorbing particles and increases with particle size.
- In future, we plan to study scattering response for large number of particles of different sizes. Results will be further utilized to get the accurate spectral signature of materials using THz-TDS.

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Thank you!