Terahertz scattering: comparison of a novel theoretical approach with experiment

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ABSTRACT

At the present time the interaction of Terahertz (THz) radiation with random structures is not well understood. Scattering effects are particularly relevant in this spectral regime, where the wavelength, and the size and separation of scattering centres are often commensurable. This phenomenon can both be used to advantage in imaging and sensing, but conversely can have adverse effects on the interpretation of a "fingerprint" spectrum. A new mathematical method, the *Phase Distribution Model,* is reported here for the calculation of attenuation and scattering of THz radiation in random materials. This uses a Phase Distribution Function to describe the effect of the non-absorbing scatterers within the media. Experimental measurements undertaken using previously published results, data obtained from specially constructed phantoms and from everyday textiles have been compared with the theory. These experimental results encompass both cylindrical and spherical scattering situations. The model has also been compared with exact calculations using the *Pendry code.*

Keywords: Terahertz, scattering, attenuation, random materials

1. INTRODUCTION

An experimental and theoretical study is reported with the objective of determining the effect of scattering of THz radiation in random structures. On the one hand, scattering has adverse effects: it may produce false signatures in spectra when interference takes place within a scattering structure (e.g. fibres in clothing or granules of powder), or diminish and scramble the return signal from a suspect item secreted below garments. On the other hand, it might be used to advantage to determine the characteristic size, texture and location of an object concealed within a matrix of other material.

An electromagnetic wave incident on a random array of scattering particles loses energy through absorption and scattering by the particles, and is thus attenuated on propagation through the scattering region. Scattered radiation may be re-scattered repeatedly leading to complete diffusion. It is prohibitively difficult to obtain exact solutions of Maxwell's equations for wave propagation in random structures; empirical approximation methods are thus needed to relate the propagation of THz to the physical properties of the material. In any practical system, used for the detection or recognition of illegal substances hidden on a suspect at some distance from the observer, this becomes especially significant. In previous work published in this area, it is evident that the theoretical approximations used often disagree with the experimental data, especially when the wave is propagating through a dense assembly of scatterers. Pearce and Mittleman [1] have determined that the statistics of a collection of scattering events provide a means to identify individual scattering events. However, when the same authors compared the mean free path for scattering through a dense collection of spheres with both exact (Mie) scattering and a quasi-crystalline approximation [2], typical differences of an order of magnitude are seen between experimental and theoretical values of the mean free path. In view of this, a mathematical procedure needs to be developed which allows the rapid prediction of the scattering and attenuation properties of an inhomogeneous material.

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We have developed a model, the *Phase Distribution Model* (PDM), which allows us to calculate the scattering and attenuation properties of an inhomogeneous material. The model proceeds by dividing the material into slices, whose thickness satisfies the following two criteria:

a) The thickness needs to be great enough so that there is no average correlation between the scatterer positions in adjacent slices, so interference effects between scattered waves for different slices will average out.
b) The slice must, conversely, be thin enough so that simple approximations for the transmission calculation can be used.

The first requirement of the model is to produce a satisfactory result for transmission of the direct beam through the sample. A *Phase Distribution Function* is used to describe the effect of the non-absorbing scatterers within the media and several approximations exist for its calculation.

Measurements reported here have been carried out using a standard broadband THz spectrometer system, as reported elsewhere [3]. Photoconductive emitters and receivers were fabricated on low temperature grown Gallium Arsenide (LT-GaAs), using electrode structures of Titanium-nickel metalization. A pulsed 20fs Ti-sapphire laser beam, centred at 780nm, of 76MHz repetition rate was used for the THz generation and detection. The beam was mechanically chopped at 1kHz and focused between the 400μm gap of the emitter's strip-line electrodes, which were biased at 200V DC. The pulsed THz radiation produced was collected, using reflection geometry [4], from the front face of the emitter and focused onto the receiver using parabolic mirrors. Detection was then carried out using a delayed pulse, split from the pump pulse, focused between bow-tie electrodes of 40μm gap size.

2. THE PHASE DISTRIBUTION MODEL

A scattering particle centred at $\underline{r} = (x,y,z)$ causes a change to both the amplitude $a(\underline{\rho})$ and phase $\varphi(\underline{\rho})$, with co-ordinate $\underline{\rho} = (x,y)$, of an incident plane wave, over some surface $z_1 > z$. The amplitude of the forward propagating unscattered wave is given by

$$F = \int a(\underline{\rho})e^{i\varphi(\underline{\rho})} \frac{d^2\rho}{W},$$

where the integral extends over the area of the wave front *W*. When calculating the attenuation of the unscattered wave, the spatial dependence of the field is not important, so the relevant information can be summarized by a phase distribution function defined by

$$P(\varphi_1) = \int_W a(\rho)\delta(\varphi(\rho) - \varphi_1)\frac{d^2\rho}{W}.$$

The unscattered amplitude is then given by

$$F = \int P(\varphi_1)e^{i\varphi}d\varphi,$$

with the transmitted intensity through the scatterer being $|F|^2$.

In this situation the distribution function becomes amenable to statistical treatment and the problem reduces to that of finding suitable approximations for its calculation. The simplest approximation for the evaluation of $\varphi(\rho)$, for a non-absorbing scatterer with refractive index n, is based on the direct projection of the optical density along the direction of propagation [5]. Evaluation of this is possible for any reasonably shaped scatterer, with a typical distribution being shown in Figure 1. By projecting the optical density of the slice onto the second surface, the phase change can be calculated for a moderate range of refractive indices.

The above method can be applied to any reasonably shaped scatterer. In the case of a sphere, of radius b and refractive index n, the phase distribution is given by

$$P(\varphi) = \frac{2\varphi}{\varphi_M^2},$$

for $0 < \varphi \le \varphi_M$, where φ_M, the maximum phase change along a path through the centre, is given by

$$\varphi_M = \frac{4\pi b(n-1)}{\lambda}.$$
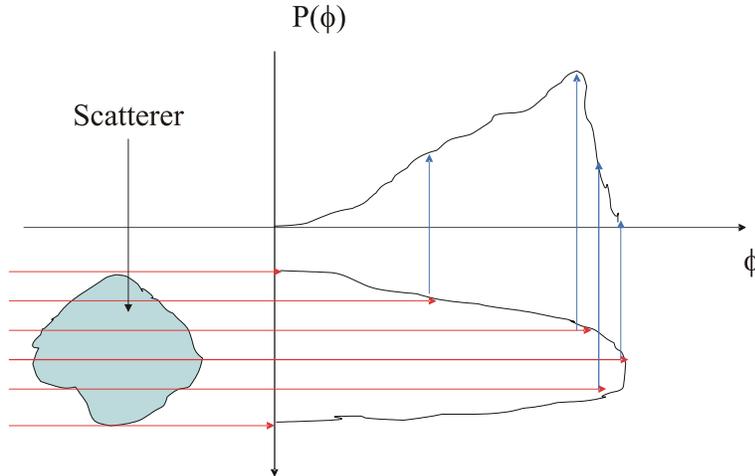

Figure 1:- Phase Distribution Projection Approximation

For an isolated object, occupying a small fraction S, of the wavefront W, the total scattering cross-section is

$$Q = 2S(1 - \int P(\varphi)\cos\varphi d\varphi).$$

This result can be used to validate the approximation methods by comparison with results from exact calculations, for example Mie theory, for cylindrical and spherical scatterers.

The model easily extends to situations involving two or more scatterers. In the case of two scattering centres, each makes an independent contribution to the attenuation and phase of the unscattered beam, provided that no correlation exists between them. In a realistic material, containing N scatterers, the transmission factor is given by

$$F = \exp\left(\frac{2\pi i d}{\lambda}\right)\left[1 - \frac{NS}{A}(1 - \int P(\varphi)e^{i\varphi}d\varphi)\right].$$

Here S is the area occupied by one scatterer of distribution function P. If the scatterers are not identical S and P are suitable averages. The mean free path for transmission through the complete material is then

$$M.F.P. = -\frac{d}{\ln|F|^2},$$

where d is the slice thickness. As stated in section 1 above, this slice thickness must be both thick enough to remove any correlation between scattering from adjacent sites and thin enough to simplify the transmission calculation through the slice.

3. COMPARISONS WITH OTHER THEORIES

The Phase Distribution Model is being compared with other theories, to test its validity. Mie theory [6] gives exact results for scattering from isolated spheres and cylinders. Comparison between the two theories shows that the model gives a good approximation if the refractive index is less than 2. Figure 2 shows the predictions of Mie theory and the Phase Distribution Model for n=1.33.
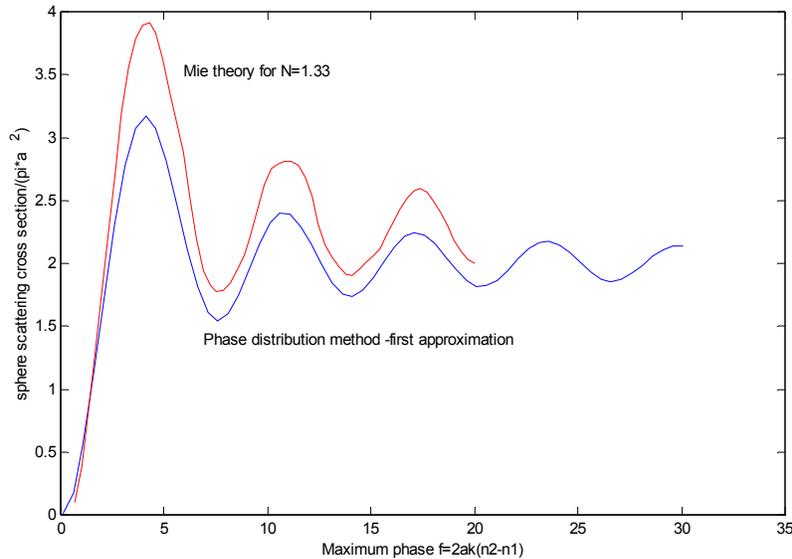

Figure 2: Normalised scattering cross section for spheres of refractive index 1.33

Comparison between exact electromagnetic calculations and the Phase Distribution Model is also being undertaken. The exact calculations are being performed on two dimensional random arrays of dielectric cylinders, using a combination of transfer matrix and multiple scattering techniques, implemented in the publicly available *Pendry Code* [7]. These calculations proceed by numerically solving Maxwell's equations using a finite-element method. A mesh of points is defined upon which the Maxwell equations are solved. Boundary conditions are set on the external plane of points in the mesh, and a transfer matrix can be defined that propagates the electromagnetic field onto the next plane of points. Such a procedure is iterated until the opposite external plane of points is reached. The transmission and reflection properties of the structure are then derived from the total transfer matrix, as described in ref. [7].

Currently good agreement is seen between the model and the exact calculations at long wavelengths. However, at short wavelengths the two results begin to diverge. Possible reasons for this may centre around the fact that the Phase Distribution Model calculates the transmitted field amplitude averaged over random scatterer positions: thus, the scattered amplitude averages to zero; but the forward wave amplitude does not. Conversely, the exact calculations determine the amplitude for a particular arrangement of random scatterers, which contains contributions from both a broad background of multiple-scattered waves and a superimposed peak from the unscattered waves. Further investigations into the discrepancies are currently in progress.

4. COMPARISON WITH EXPERIMENT

Currently, transmission data from a number of scattering experiments is being compared with the Phase Distribution Model's predictions. Propagation of THz through random cylindrical and spherical scattering structures has been investigated, as have the attenuating properties of cloth.

4.1 Spherical Scatterers

Mittleman and co-workers [2] have previously reported the mean free path of THz radiation through collections of randomly arranged Teflon spheres. The internal path lengths of the scatterers varied from 1.19mm to 20.64mm and encompassed a variation in the mean free path of a factor of 40. As noted in section 1 above, they have compared their results with theories based on Mie theory and a quasi-crystalline approximation and found that neither of the two treatments gives a satisfactory fit to the data. The Phase Distribution Model has been compared with this data and found to give a much closer fit to the measured signal attenuation. Figure 3 shows comparison of the data with the results from the PDM calculations. The general trend of the data is well described, but the pair distribution function introduces oscillations which are not included.
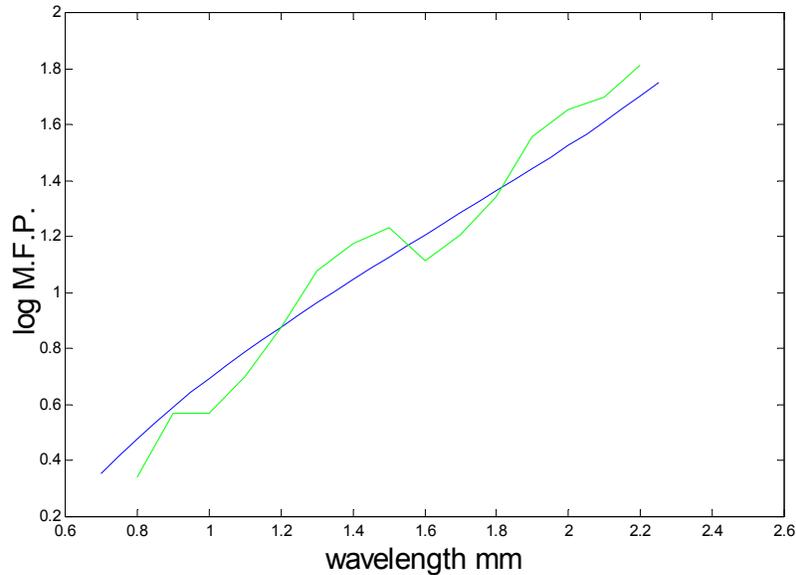

Figure 3:- Phase Distribution Model prediction of THz attenuation in random spheres.

4.2 Cylindrical Scatterers

Specially constructed phantoms of dielectric cylinders have been fabricated at Durham and the THz transmission through them investigated.   These phantoms are made from the UV-curable resin Si-50, which has a refractive index of n=1.65±0.05 in the range of 0.2 – 3THz, using a stereolithographic process. The phantoms are of varying volume concentration, ranging from 10% to 50%, each containing a number of randomly placed identical cylinders; the cylinder diameter is varied from phantom to phantom, in the range of 0.4mm to 1.0mm, whilst their height is constant at 10mm. Figure 4 below shows a birds-eye view of one such phantom.
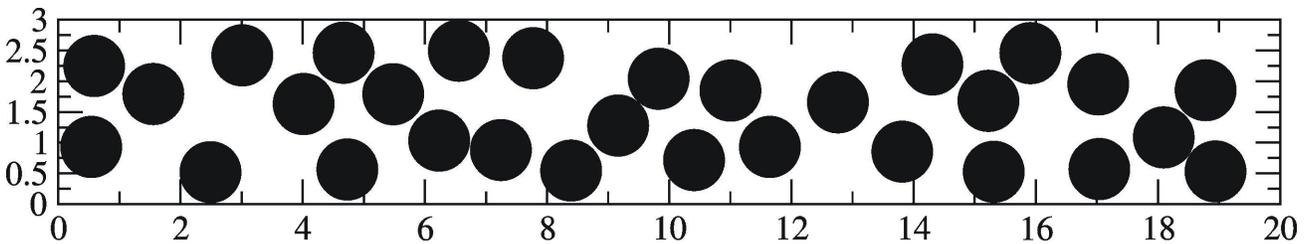

Figure 4:- Birds eye view of a cylindrical scattering structure.
Scatterer concentration 40%, cylinder diameter 1.0mm

Comparison of the experimental data with the PDM predictions is looking promising. Currently only high volume fraction phantoms have been constructed and tested (40% and 50% concentration). Figure 5 shows the data obtained

from a random structure, with a scatterer volume fraction of 50% and diameter 0.4mm. Figure 6 is the equivalent plot for cylinders of diameter 1mm and volume fraction 40%, the phantom structure shown in Figure 4.

Both sets of data have regions of high and low transmission in the frequency spectrum. The attenuation dips arise because of interference between directly propagating THz radiation, which has passed straight through the structure without taking part in a scattering event, and THz radiation which has been multiply scattered on passing through the phantom and has thus emerged at an angle equivalent to its incident angle. Comparison of the experimental data with the Phase Distribution Model's predictions shows that areas of high and low absorption are expected. The expected frequencies of these features are well matched between theory and experiment: for example 0.7THz in the 50% volume scatterer and 0.3THz for the 40% structure. The order of magnitude of absorption for certain frequency peaks is also in good agreement.
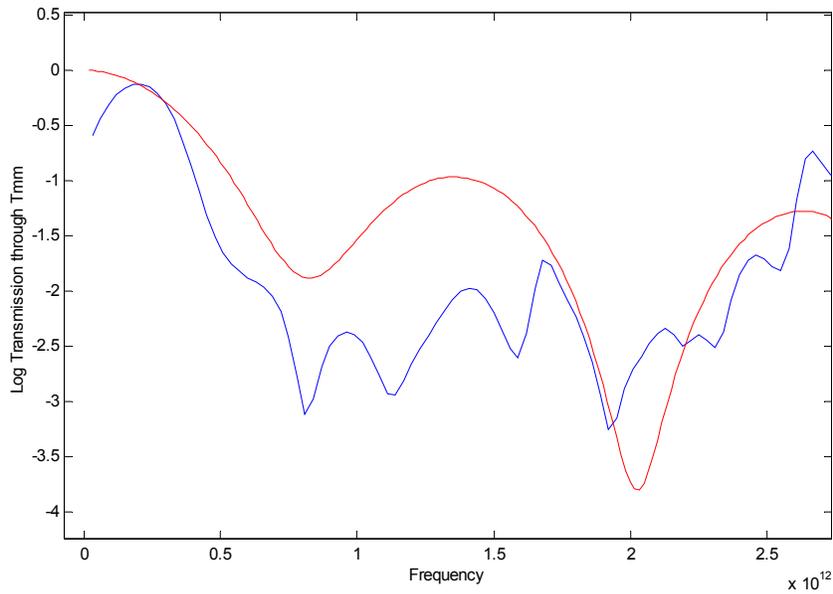

Figure 5:- THz transmission through a random array of cylinders
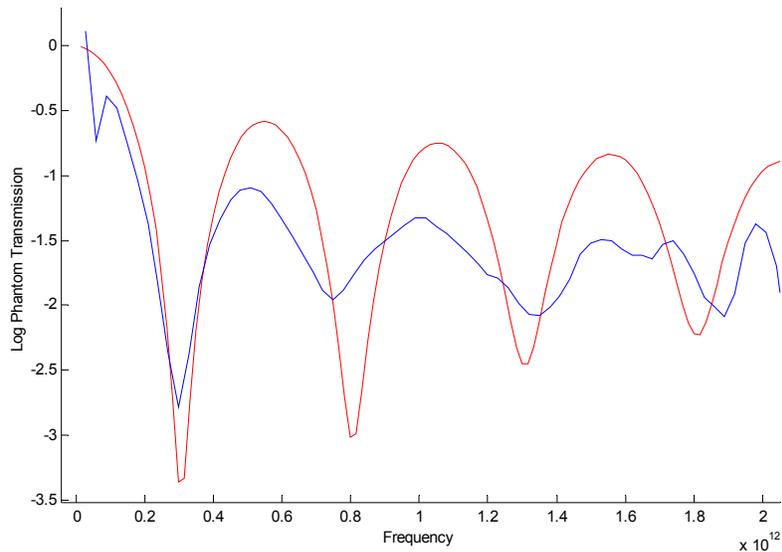Scatterer concentration 50%, cylinder diameter 0.4mm

Figure 6:- THz transmission through a random array of cylinders
Scatterer concentration 40%, cylinder diameter 1.0mm

4.3 Clothing Fabrics

Terahertz transmission measurements through clothing have been carried out both at Durham and by other workers [8]. The required parameters of the model are the sizes and spacings of the yarns in the cloth, which can be obtained using scanning tunnel microscopy and the effective refractive index of the material, an empirical parameter. The yarns of the cloth are assumed to be uniform cylinders, made from fibres that are too small to be resolved in the THz regime. Once again the projected optical density [5] is used for the phase change calculation. Figure 7 below shows the THz attenuation through a piece of cotton shirt, with effective refractive index n=1.29. The yarn diameters in the shirt are 180 microns, whilst the spacings are 330 microns and 250 microns for the warp and weft respectively. The THz absorption of the shirt is seen to increase with frequency in good agreement with the model's prediction. Fits to other data [8] indicate that the model is suitable for describing attenuation in a number of different fabrics, including cotton, polyester and terylene.
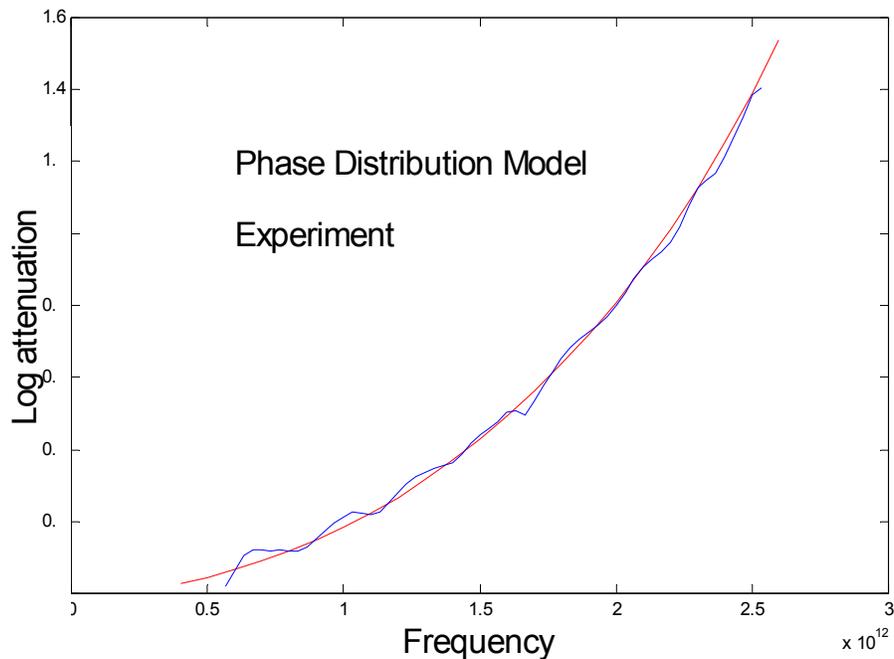
Figure 7:- THz transmission through a cotton shirt, with the PDM prediction

5. PHASE DISTRIBTUION MODEL FOR SCATTERING

The Phase Distribution Model can be extended to describe the angular dependence of the scattered radiation. A knowledge of THz transmission through the random structure is required before this can be calculated. Within a random structure the number of scattering events depends on its relative thickness and the mean free path of the radiation through the structure. A short mean free path compared to sample thickness indicates that multiple scattering events will take place implying diffusion of the radiation, whereas a long mean free path means that first ordering scattering will dominate throughout the volume. The optical projection method for determining the unscattered amplitude can be adapted for the scattering calculation. If the spatial variation of amplitude and phase over the second surface of a slice is known, the amplitude of the forward scattered waves can be found by using the method of the angular spectrum of plane waves [5]. It follows that the scattered intensities are related to the spatial correlation of the emerging field. For direct forward transmission this was found by the approximation method of projecting the optical density along the propagation direction. For scattering, it appears to be an appropriate approximation to project the optical density along a direction intermediate between the incident and scattered directions.

In order to test this idea, calculations have been performed of the scattering by a dielectric cylinder, and the results compared with the exact solutions of the wave equation. Figure 8 shows that satisfactory agreement is obtained for a moderate range of refractive indices (n < 2), which supports the use of this approximation for more complicated structures that are not amenable to exact calculation.
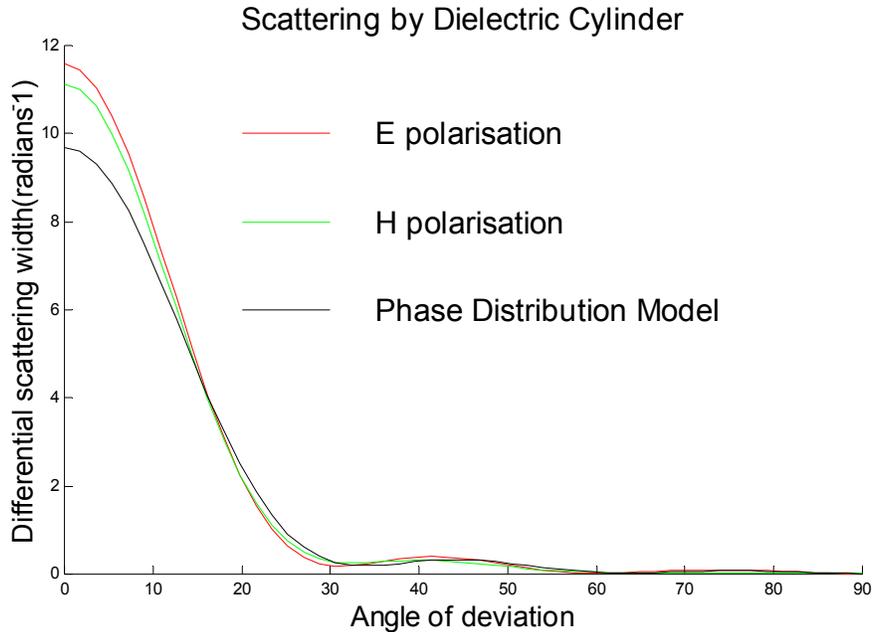
Scattering by Dielectric Cylinder

Figure 8:- Phase Distribution Model with oblique projection

6. CONCLUSIONS

The Phase Distribution Model has been found to provide a good description of the propagation of waves through random media. Comparison with exact theory has shown that the model provides a suitable description of the expected scattering from isolated cylinders and spheres over a range of refractive indices (n < 2). Experimental tests of the model have also indicated that it describes the forward propagating THz attenuation in random structures of varying volume concentrations and scatterer size, as well as providing a good description of the THz attenuation through regularly arranged fabrics. Early indications are also promising for the model's ability to describe the scattering of THz radiation from randomly arranged structures.

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