A SCATTEROMETER FOR OPERATION FROM 50 TO 750 GHZ

Roger Appleby (1), Richard Wylde (2), Stuart Froud (2), Per Heighwood Nielsen(3), Cecilia Cappellin(3), Philip Atkin(4) and Elena Saenz(5)

(1) *Roger Appleby MMW Consulting Ltd, 60 Churchill Drive, Malvern Link, Worcs, WR14 1DJ, UK,*

Email: applebyroger@yahoo.co.uk

(2) *Thomas Keating Ltd, Station Mills, Daux Road, Billingshurst, West Sussex, RH14 9SH, UK*

(3) *TICRA, Landemærket 29, DK-1119, Copenhagen, Denmark*

(4) *Pixel Analytics Ltd, 93A New Road, Haslingfield, Cambridge CB23 1LP, UK*

(5) *ESA/ESTEC, Keplerlaan 1, PO Box 299, 2200 AG Noordwijk ZH, The Netherlands*

***Abstract* – A scatterometer operating in the bands from 50 to 750 GHz has been designed and fabricated. Operation in the different bands is achieved by using a Network Analyser with appropriate frequency extenders and corrugated horns. The beam is propagated using reflective quasi-optics on two levels with the sample being mounted on the lower level. The two levels are joined by a rotating periscope which collects the scattered radiation from the sample and transfers it to the upper base plate were the phase and amplitude are measured by the Network Analyser. The scatterometer can measure in reflection and transmission and in all 4 linear polarisations. During a measurement the network analyser heads and associated cables remain static to prevent phase drift. The scatterometer can determine sample roughness and use this data to calculate the transmission and reflection coefficients of an equivalent smooth sample. Prototype rough reference samples have been developed for testing the scatterometer.**

I. Introduction

Many different materials including composites are used in the field of antennas. Examples include dielectrics, frequency selective surfaces (FSS), sandwich structures, composite resins, ceramics and metal plates which can be seen in applications ranging from low frequencies up to sub-mm waves. An accurate characterization of these materials is of vital importance for future missions in the Telecom, Earth Observations and Science domains.

A common way of describing these materials is in terms of reflection, transmission and absorption. This is sufficient in the case of homogeneous materials with perfectly flat and smooth interfaces. When the material is inhomogeneous or rough, however, some of the incoming radiation will be scattered away. To measure this scattering and therefore improve the measurement of reflection, transmission and absorption a scatterometer has been designed and fabricated to operate in the 50 -750 GHz region of the spectrum.

A feasibility study was conducted to down select the best design against the following key requirements:

1. The design should build on the existing Thomas Keating Bench and Network Analyser(PNA) extenders in bands from 50-750 GHz
2. The Network analyser heads should remain static to avoid phase drift due to cable movement
3. For metals determine the reflection coefficient
4. For dielectrics/magnetic materials extract the permittivity and permeability
5. Provide suitable calibration methodology
6. Measure the scattered radiation from rough samples
7. Provide reference surfaces for smooth and rough samples

A design was selected based on a rotating periscope previously reported by Lo et al.[1] which rotates around the sample enabling the network analyser extenders and associated cables to remain static. This paper reports on the research and development to convert the feasibility study to a working instrument. Section II describes the scatterometer and section III the software which also incorporates the calibration and extraction of permittivity and permeability for dielectrics and magnetic materials. Section IV discusses reference samples and section V provides a summary and conclusions.

II. SCATTEROMETER

A block diagram of the scatterometer is shown in Figure 1. The system consists of an optical bench which presents the incoming beam to the sample and collects the reflected, transmitted and scattered radiation. The incidence angle and the scattered angle are controlled by the computer through a motion controller. The same computer also interfaces with the network analyser defining the frequency and power of the beam arriving at the sample and collecting from the network analyser the radiation received from the sample. The computer uses MATLAB and its Instrument Control toolbox to achieve this. Measured data can be displayed and analysed and predictions of scattering can also be made. The software is discussed in more detail in section III and the quasi optic bench and sample holder are described below.

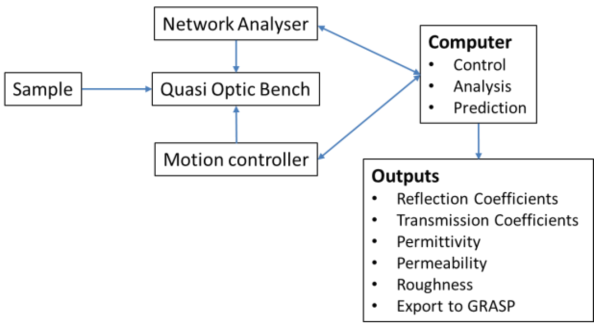

Figure 1 Scatterometer Block Diagram

A. Quasi Optic Bench

The bench is based on a two levels as shown in Figure 2 with an upper and lower baseplate.

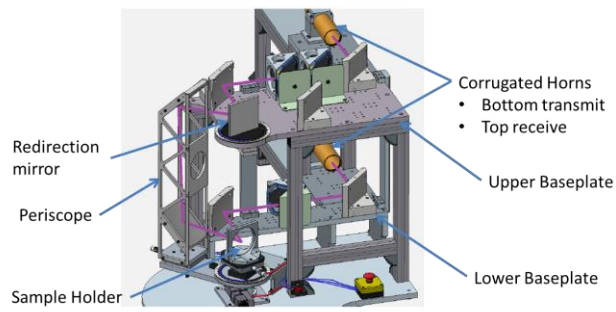

Figure 2 Quasi Optic Bench

Radiation from the network analyser enters the optical system through the corrugated horn on the lower base plate and is relayed onto the sample using ellipsoidal mirrors. The beam launched from the corrugated horn has its electric vector inclined at 45 degrees so that the polarisation of the beam can be set vertical or horizontal with respect to the baseplate by using a pair of wire grid polarisers. The sample holder is described in section B and provides all the necessary adjustments to align the sample which can also be rotated under computer control to vary the incidence angle.

Radiation reflected, transmitted or scattered from the sample is collected by a periscope comprising of two paraboloid mirrors. To provide measurements at different angles the periscope can rotate around the sample under computer control. It relays the light from the lower baseplate to the upper baseplate and is constructed from a dielectric material to avoid reflections. It is also mounted on a precision translation stage to allow the distance to the sample to be varied providing a line calibration (see section III A).

Once on the top base plate the first element is a plane redirection mirror which tracks the periscope redirecting the beam in to either the reflected path shown in Figure 2 or the transmitted path. The transmitted path sends the beam to the mirror to the right of the redirection mirror and the load (shown in green) has to be removed and placed in the reflect path. The orientation of the first polariser also has to be changed so that it will reflect the beam to the receive horn. The polarisers are identical to the ones on the lower base plate and allow selection of either vertical or horizontal polarisation. The electric vector enters the corrugated horn at 45 degrees.

The PNA heads, extenders and cables remain static at all times during measurements and this will provide excellent stability and repeatability. The grid arrangement on the upper and lower base plates will also reduce standing waves which again will give rise to more stability.

Detailed simulation of the optical design was completed using GRASP and several improvements to the design were made and are reported in a separate paper at this workshop[2].

B. Sample Holder

The scatterometer incorporates a precise mechanism for positioning and aligning the sample as shown in Figure 3. There is a large flat reference surface to attach the sample to using either rubber bands or clips or bespoke fastenings. This reference surface can be adjusted in three different ways. First it can be tilted to correct for parallelism errors in the sample, second it can be translated to ensure the axis of rotation passes directly through the reference plane of the sample and third it can be rotated.

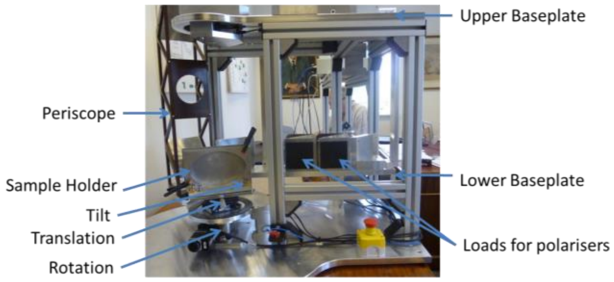

Figure 3 Scatterometer side view showing sample holder

Rotation of the sample is used to set the incidence angle but any wedge shaped error in the sample can be corrected by application of a simple offset.

There are three sample holder adaptor plates with different apertures, 110, 85 and 55 mm with the smaller two being circular and the 110 one shown in Figure 3 elliptical to facilitate a larger range of angles in transmission.

C. Network analyser, extenders and corrugated horns

The Network Analyser used is a Keysight[1] N5224A It can operate in the bands shown in Table 1 with VDI[2] extenders. To access each band the extenders have to be physically changed.

Table 1 Network Analyser Extenders

Frequency GHz		
Start	**Stop**	**S parameters**
50	75	S_{11},S_{21}
75	110	S_{21}
110	170	S_{21}
170	260	S_{21}
220	330	S_{21}
330	500	S_{21}
500	750	S_{21}.

In frequency bands that just measure one S parameter (labelled as S_{21} in Table 1) the scatterometer can be configured to either measure in transmission for S_{21} or measure in reflection for S_{11}. If the sample is a symmetric network then $S_{11}=S_{22}$ and $S_{21}=S_{12}$ which is the case for most dielectric samples.

The beam is launched into free space using an ultra-Gaussian corrugated horn[3] with a separate horn for each band.

III. SOFTWARE

The software is written in MATLAB[3] and uses the Instrument Control toolbox for accessing the PNA. The system is operated from a tabbed Graphical User Interface and provides all the functions and associated processes required to run the scatterometer including comprehensive help files. The main tabs are:

- Measure, further divided into:
  - Details
  - Acquire
  - Analyse
- Predict

An overview of each is given below drawing attention to novel features.

A. Measure

The measure tab provides the input for running all measurements including experimental description, incidence and scattering angles, frequency range, whether the sample is metal or dielectric and a choice of calibration methods. This data defines the workflow to be followed. During acquisition prompts to the user are provided to configure the instrument suitably to record sample and calibration data.

The calibration for reflected samples is provided by reference to a smooth metal surface with known reflectivity (see section IV). For dielectrics two methods reported by Will and Rolfes[4-6] are used. In both cases it is assumed that the sample is a symmetric network. The simple error model shown in Figure 4 is used with the error two port networks **A** and **B** and the transmission matrix $\mathbf{T}_{DUT}$ of the respective measuring object.

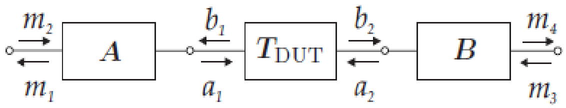

Figure 4 Error Model

This results in the measuring matrices **M** (see equation 1-3) at the actual frequency (f_i) for the calibration standards T, and L and the sample N with the respective transmission matrices T_T, T_N, and T_L.

$$\mathbf{M}T(f_i) = \mathbf{A}(f_i) \cdot \mathbf{T}_T(f_i) \cdot \mathbf{B}(f_i) \quad 1$$

$$\mathbf{M}L(f_i) = \mathbf{A}(f_i) \cdot \mathbf{T}_L(f_i) \cdot \mathbf{B}(f_i) \quad 2$$

[1] http://www.keysight.com

[2] https://vadiodes.com/en/

[3] https://uk.mathworks.com/products/matlab.html

$$\mathbf{M}R(fi) = \mathbf{A}(f_i) \cdot \mathbf{T}_N(f_i) \cdot \mathbf{B}(f_i) \quad 3$$

$$\mathbf{M}L,syn(f_i) = \mathbf{A}(fi + \Delta f) \cdot \mathbf{T}_{L,syn}(f_i) \cdot \mathbf{B}(f_i + \Delta f) \quad 4$$
$$= \mathbf{A}(f_i + \Delta f) \cdot \mathbf{T}_T(f_i + \Delta f) \cdot \mathbf{B}(f_i + \Delta f)$$

These equations can be solved using standard techniques to give the calibrated reflection and transmission Coefficient. The line standard is achieved using the translator under the periscope as described in section IIA. The line length should be changed by a quarter of a wavelength at the highest frequency. This algorithm is known as the Through, Line, Network (TLN) and there is a similar algorithm which uses a synthetic line know as the Through, Through, Network (TTN). To use the TTN algorithm equation 2 for the real line is substituted by equation 4 which is a synthetic line. The synthetic line is a Thru at (fi +Δf) with Δf providing the phase shift. The frequency interval needs to be selected such that a phase shift of >20 and <160 degrees[7] is achieved by Δf and the measured data needs to be relatively smooth.

B. Analyse

For a dielectric/magnetic material once calibrated S parameters have been obtained t several methods are available for extracting the permittivity and permeability which include:

- Nicholson Ross Weir[8, 9]
- Add-Unwrap[10]
- Luukonen[11]
- Iterative[12]
- Ellipsometry[13, 14]
- Duvillaret[15]

These methods have different strengths and weaknesses some can extract both permittivity and permeability whilst others can only extract permittivity. In all cases the problem is how to handle the multiple branches in the transmission coefficient i.e. when the phase passes through 2π it returns to zero producing a new branch. Nicholson Ross Weir uses an integer to select which branch should be used, whilst Add-unwrap attempts to unwrap the transmission coefficient prior to further analysis. Luukonen is a stepwise Nicholson Ross Weir algorithm which uses adjacent points to overcome branching issues. The iterative method uses a fitting process varying the estimated material parameters to give the best fit to the measured data and is best used to refine results. Ellipsometry requires collection of the specular reflection in vertical and horizontal polarisations at different angles of incidence from this data the permittivity can be extracted. The Duvillaret method can also be used to extract permittivity and only requires one polarisation.

To test these extraction methods analytical data was generated for a 0.617 mm thick piece of alumina with dielectric constant = 9.2, a tan δ = 1.7×10^{-3} and a permeability of 1 using the method described by Kanieckie et al.[16]. Analytical data was also generated for the Through and Line components assuming the sample is at the centre of a 1 m air path which is approximately equivalent to the scatterometer path length and the loss of the air was set to 0.2 np/m. This data was then calibrated using one of the techniques discussed in section A and then the permittivity and permeability extracted as shown in Figure 5.

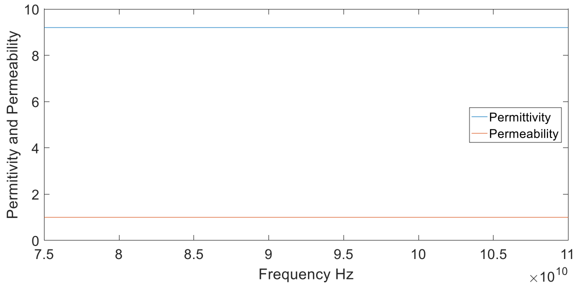

Figure 5 Permeability and permittivity using Add-Unwrap and TLN calibration method

It can be seen that, in the absence of noise the permeability and permittivity are extracted accurately.

The variation of the specular response either in transmission or in reflection due to the presence of a rough surface can be measured as a function of frequency, angle and polarisation. This data can in turn be used to estimate the reflectivity or transmission of a sample as if it were smooth and to give an estimate of the surface roughness. This is achieved by fitting a simple model based on Total Integrated Scatter and is similar to the method used to quantify roughness of semiconductor wafers[17].

The scatterometer also has the ability to measure transmitted and reflected scatter and use this information to calculate the Power Spectral Density (PSD) of the surface which in in turn can be used to calculate the Auto Covariance Function (ACF). Knowledge of the surfaces physical properties in the form of the ACF provide a method to correct S parameters measured with rough surfaces to what they would have been had the surface been smooth.

C Predict

The predict tab provides two method for predicting scattering using either the Generalised Harvey Shack method [18] for an interface between two media or using the Radiative Transfer Method [19] for volume scattering.

In both cases the input includes the frequency (or wavelength), the angle of incidence and the dielectric constant of the media. The Generalised Harvey Shack method uses the ACF of the surface whilst the Radiative Transfer method requires a description of the scatterers in the medium.

The Generalised Harvey Shack method can take as an input the ACF extracted from a measurement and can this can then be used to extrapolate scattering data to a different wavelength or incidence angle. This is only possible if the wave front arriving from the sample is approximately flat.

IV. REFERENCE SAMPLES

To determine that the scatterometer is working correctly some reference samples are required. ESA already has smooth reference samples as shown in Table 2.

Table 2 Smooth Reference samples

Reference material	**Roughness nm RMS**
Aluminium	50
Copper	50

These metal surfaces are used to provide the required reflect reference.

To fully evaluate the scatterometer rough reference surfaces are required with properties which are known in both reflection and transmission. In the infrared and millimetre wave region engineered surfaces have been used to achieve this [20, 21]. That is the surface is manufactured with known properties. In the lower millimetre wave bands (~100 GHz) these surfaces have been machined using numerically controlled milling machines[20].

A surface with a Gaussian distribution was selected with a correlation length and roughness such that scattered radiation was above the noise floor of the scatterometer. The initial analysis was done with GRASP as part of demonstrating the feasibility of the optical design and later the surface properties were refined using the Generalised Harvey Shack method. An example of the results from the GRASP analysis for the scatterometer working at 62.5 GHz is shown in **Error! Reference source not found.**. Here the black curve is the output from the scatterometer with a smooth sample and the red the output from a rough sample with a Gaussian distribution having a roughness (σ_{RMS}) = 0.23 mm and a correlation length (Cl) = 3.86 mm.

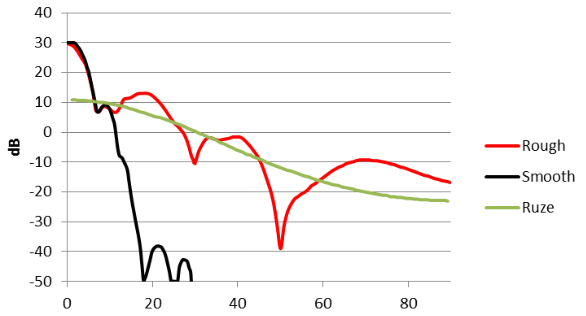

Figure 6 GRASP Prediction, 62.5GHz, σ_{RMS} =0.23, Cl=3.86 mm

These values were refined to give the surfaces for use as shown in **Error! Not a valid bookmark self-reference.** at 62.5GHz and 400 GHz.

Table 3 Reference surfaces at 62.5 and 400 GHz

Material	Frequency GHz	Correlation Length mm	σ_{rms} mm
Metal	62.5	3.86	0.1
Dielectric	62.5	3.86	0.23
Metal	400	0.386	0.023
Dielectric	400	0.386	0.138

These surfaces can be designed using the method of Thorsos which introduces a random element into the PSD of the surface. The amplitude of the PSD is convolved with a complex random number to provide the ordinates (z) of the surface. The convolution is normally conducted using a Fast Fourier Transform with the amplitude of the PSD being multiplied with a random number before transform. Care has to be taken to ensure the boundary conditions are correct and the function remains real and symmetric[22].

At 62.5 GHz the dimensions are such that the surfaces can be machined with a small ball end cutter (0.5 mm) and the dielectric and metal surface are shown in Figure 7.

Figure 7 Rough Reference samples 62.5 GHz. Left aluminium, right Dielectric

At 400 GHz the dimensions are such that conventional machining is not possible as the dimensions are reduced by ~x10 and the cutter required is physically too small. To machine these surfaces a laser machining process at

University of Birmingham[4] was used and the result of the first sample produced in stainless steel to demonstrate feasibility is shown in Figure 8.

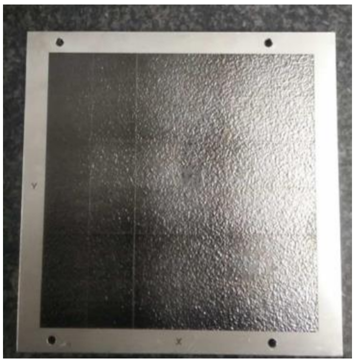

Figure 8 Rough Reference sample 400 GHz

The surface is black as it is covered in a thin coating of oxide. This sample was machined in 20 mm squares and the outlines of the squares can be seen in the figure.

A Coordinate Measuring machine (CMM) confirmed that the 62.5 GHz samples are within 1μm of the designed profile whilst at 400 GHz a focus variation microscope was used to confirm that the surface roughness and correlation length are within acceptable limits. This sample will be evaluated on the scatterometer prior to machining the surface and also machining the dielectric.

V. Conclusions

A scatterometer capable of measuring both specular and diffuse transmission and reflection from 50 – 750 GHz has been designed and manufactured. It is based on a two level quasi optical bench and uses a periscope to rotate around the sample which allows the network analyser and extenders to remain stationary. The beams are generated by ultra-Gaussian corrugated horns and a different set of extenders and corrugated horns are required for each band.

The instrument is controlled by software and is capable of producing calibrated measurements which can then be used to calculate the permittivity and permeability of dielectric/magnetic samples. The angular response of the calibrated data can be used to correct specular transmission and reflection for roughness and in turn to determine what that roughness is. This data can also be imported into GRASP.

The reference samples will provide a means of evaluating the scatterometer and testing its performance against samples with known properties. The rough samples will also provide a means of evaluating the performance of the scattering models discussed under the predict section

VI. Acknowledgement

We would like to acknowledge support from ESA under contract 4000116424.

VII. REFERENCES

[1] S.-Z. A. Lo, D. Novotny, E. N. Grossman, and E. J. Heilweil, Pulsed terahertz bi-directional reflection distribution function (BRDF) measurements of materials and obscurants in *Passive Millimeter-Wave Imaging Technology XIV* Proc. SPIE *8022*, 2011.

[2] R. Appleby, P. Heighwood Nielsen, C. Cappellin, R. Wylde, S. Froud, and E. Saenz, Simulation and design of a scatterometer for the THz region, presented at the *38th Antenna Workshop*, Noordwijk, Netherlands, 2017.

[3] R. Wylde. (31 August 2017). *Ultra Gaussian Corrugated Horns*. Available: http://www.terahertz.co.uk/index.php?option=com_content&view=article&id=189&Itemid=563

[4] B. Will and I. Rolfes, A new approach on broadband calibration methods for free space applications, in *Microwave Symposium Digest (MTT)*, 2012, pp. 1-3.

[5] B. Will and I. Rolfes, Application of the thru-network-line self-calibration method for free space material characterizations, in *International Conference on Electromagnetics in Advanced Applications (ICEAA)*, 2012, pp. 831-834.

[6] B. Will and I. Rolfes, A synthetic calibration technique for broadband applications using focusing antenna setups, in *Antennas and Propagation Society International Symposium (APSURSI)*, 2013, pp. 722-723.

[7] B. Will and I. Rolfes, The TTN-method - A phase shift calibration technique for vector network analyzers, in *Asia-Pacific Microwave Conference 2011*, Asia-Pacific Microwave Conference 2011

2011, pp. 697-700.

[4] The author acknowledge the work of Dr Pavel Penchev, Mechanical Engineering Department for preparing this sample.

[8] E. J. Rothwell, J. L. Frasch, S. M. Ellison, P. Chahal, and R. O. Ouedraogo, Analysis of the Nicolson-Ross-Weir Method for Characterizing the Electromagnetic Properties of Engineered Materials, *Progress In Electromagnetics Research*, vol. 157, pp. 31-47, 2016.

[9] W. B. Weir, Automatic measurement of complex dielectric constant and permeability at microwave frequencies, in *Proceedings of the IEEE*, *62*, 1974, pp. 33-36.

[10] J. J. Barroso and U. C. Hasar, Resolving phase ambiguity in the inverse problem of transmission /reflection measurement methods, *Journal of Infrared, Millimeter, and Terahertz Waves*, vol. 32, 2011.

[11] O. Luukkonen, S. I. Maslovski, and S. A. Tretyakov, A Stepwise Nicolson-Ross-Weir-Based Material Parameter Extraction Method, presented at the *Antennas and Wireless Propagation Letters, IEEE*, 2011.

[12] A. International, ASTM D5568-1: Standard Test Method for measuring Relative Complex permittivity and Relative Magnetic Permeability of Solid Materials at Microwave Frequencies, ed. 100 Barr Harbor Drive, PO Box C700, West Conshohocken, PA 19428-2959, United States: ASTM, 2001.

[13] F. Sagnard, F. Bentabet, and C. Vignat, In situ measurements of the complex permittivity of materials using reflection ellipsometry in the microwave band: theory (Part I), *IEEE Transactions on Instrumentation and Measurement*, vol. 54, pp. 1266-1273, 2005.

[14] F. Sagnard, F. Bentabet, and C. Vignat, In situ measurements of the complex permittivity of materials using reflection ellipsometry in the microwave band: experiments (Part II), *IEEE Transactions on Instrumentation and Measurement*, vol. 54, pp. 1274-1282, 2005.

[15] L. Duvillaret, F. Garet, and N. B. Crane, Highly precise determination of optical constants and sample thickness in terahertz time-domain spectroscopy, *Applied Optics*, vol. 38, pp. 409-415, 1999 1999.

[16] M. Kaniecki, E. Saenz, L. Rolo, R. Appleby, and O. Breinbjerg, Scattering-Parameter Extraction and Calibration Techniques for RF Free-Space Material Characterization, in *8th European Conference on Antennas and Propagation (EUCAP)*, 2014.

[17] Test method for measuring reflective total integrated scatter (TIS), SEMI Standard MF1048-1111, 2012.

[18] A. Krywonos, J. E. Harvey, and N. Choi, Linear systems formulation of scattering theory for rough surfaces with arbitrary incident and scattering angles *Journal of the Optical Society of America A-Optics Vision*, vol. 28, pp. 1121-1138, Jun 2011.

[19] K. M. Nam, L. M. Zurk, and S. Schecklman, Modeling terahertz diffuse scattering from granular media using radiative transfer theory, *Progress In Electromagnetics Research B*, 2012.

[20] P. Phu, A. Ishimaru, and Y. Kuga, Copolarized and cross-polarized enhanced backscattering from two-dimensional very rough surfaces at millimeter wave frequencies, *Radio Science*, vol. 29, pp. 1275-1291, 1994.

[21] K. A. O'Donnell and R. Mendez, Experimental study of scattering from characterized random surfaces, *J. Opt. Soc. Am. A*, vol. 4, pp. 1194-1205, 1987.

[22] C. A. Mack, Generating random rough edges, surfaces, and volumes, *APPLIED OPTICS* vol. 52, March 2013 2013.