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# Study on the Variation in Dielectric Properties of Heterogeneous Substrates Composed of Nanomaterials

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**Abstract**— An analytical study of heterogeneous substrates created by including small particles arranged in a cubic lattice within a host medium is presented in this paper. Rapid advances in nanomaterial fabrication techniques will allow in the near future, heterogeneous samples to be created with nano or micro-sized inclusions, and this paper investigates the electromagnetic (EM) properties of these structures. Analytical equations by various authors for the effective permittivity and permeability of such artificial materials have been analysed and compared over microwave frequencies. The particle size, spacing and frequency were examined individually to understand their role in determining the effective EM parameters of the heterogeneous mixture. Furthermore, results from FDTD simulations with micro-sized cuboids were processed using an inverse scattering algorithm to obtain the effective permittivity and permeability of these heterogeneous structures using a complimentary technique. The canonical formulations showed reasonable agreement with the EM simulations and the two methods can be used to design novel dielectric substrates.

## I. INTRODUCTION

The concept of altering the properties of a medium by including particles of different electromagnetic (EM) properties in various lattice configurations to form a heterogeneous material has been of considerable interest to material and antenna engineers [1-9]. This can potentially allow the ‘creation’ of new materials that possess novel and bespoke dielectric properties.

Reference [1] can form a basis for different heterogeneous structures with tailored EM parameters (notably highly conducting or highly dielectric). Nanomaterial fabrication technology is developing at a rapid rate and we envisage that it will soon be possible to integrate these novel substrates with conducting sections to form complete antennas and circuits which can be produced in one process. By making larger structures (~mm) out of nano-particles (metallic and/or non-metallic), resonances at microwave frequencies are possible [9]. Physical and fabrication advantages include potentially faster fabrication processes and reduced production costs. Novel and customised substrate properties are also made possible, by controlling the particles’ volume ratio. EM advantages – bandwidth, size and efficiency – are achievable by smoothly varying the permittivity with electric field

strength location, or creating substrates with equal permittivity,  $\epsilon$  and permeability,  $\mu$ .

This paper compares the theoretical analyses by different authors in this field of study to obtain a suitable canonical formulation for heterogeneous structures. Results from EM simulations of different structures are then analysed for comparison with the results from the mathematical formulations. These solutions will be the starting point for future work to achieve artificial materials using nanomaterials suitable for microwave frequencies. Note that throughout this paper the permittivity and permeability values are the relative values and must be multiplied by the respective free space constants.

## II. THEORETICAL ANALYSIS

Lord Rayleigh was the first to examine how the properties of a medium are modified when obstacles are placed in it [2]. But the analysis by Lewin in [1] is more often cited, and so forms a strong background for investigating heterogeneous substrates. A general mathematical expression for the EM properties of particle-embedded mixtures is given in [3] as

$$K_{\text{eff}} = K_1 \frac{[(K_2 + 2K_1)(K_1 - K_2)^{-1}] - 2f + C(K_1, K_2, f)}{[(K_2 + 2K_1)(K_1 - K_2)^{-1}] + f + C(K_1, K_2, f)} \quad (1)$$

where  $K_1$ ,  $K_2$  and  $K_{\text{eff}}$  are the appropriate parameters of the host medium, the inclusions (in its bulk form) and the mixture respectively;  $f$  is the total volume fraction of the inclusions.  $C(K_1, K_2, f)$  represents corrections for higher-order multipole terms as a result of the decomposition of the scattered field [1, 10].

Different authors have previously proposed equivalent versions of equation (1) and the differences will be compared below. Lewin in [1] does not have the correction term, approximates Stratton’s equations in [10] for scattering of EM waves by using a sphere and assumes the particles are in a cubic lattice in a semi-infinite medium. Doyle [4] and Cai et al [5] use similar equations as both use the exact equations derived in [10] to obtain the  $n$ th order magnetic and electric scattering coefficients of the particles and the Clausius-Mossotti equations for the effective permittivity and permeability of the heterogeneous structures,  $\epsilon_{\text{eff}}$  and  $\mu_{\text{eff}}$ .

However, they represent the dipole polarisabilities of a sphere differently, and the EM properties of the host medium ( $\epsilon_1, \mu_1$ ) is accounted for in [4] but not in [5]. In [6], the inclusions examined are conducting and an interaction constant between the particles is defined, which is used in its representation of the Clausius-Mossotti equations. Common to [6] and [7] is the absence of frequency terms in their analyses. Reference [8] extends the analysis in [7] such that the EM properties of the inclusions differ from each other in electric and magnetic resonance modes represented by spheres of different radii but from the same material. The differences in the representation of the effective  $\epsilon$  and  $\mu$  by these authors are explained in the following section.

The equations for the effective  $\epsilon$  and  $\mu$  from [1] are:

$$\mu_{eff} = \mu_1 \left( 1 + \frac{3f}{\frac{\mu_p + 2\mu_1}{\mu_p - \mu_1} f} \right); \quad \epsilon_{eff} = \epsilon_1 \left( 1 + \frac{3f}{\frac{\epsilon_p + 2\epsilon_1}{\epsilon_p - \epsilon_1} f} \right) \quad (1)$$

where  $f = \frac{4}{3}\pi a^3/s^3$ ,  $a$  is the sphere's radius,  $s$  is the particle's spacing, ( $\epsilon_p, \mu_p$ ) are the effective values of the particles given by:

$$\frac{\epsilon_p}{\epsilon_2} = \frac{\mu_p}{\mu_2} = \frac{2(\sin\theta - \theta\cos\theta)}{(\theta^2 - 1)\sin\theta + \theta\cos\theta} = F(\theta)$$

where ( $\epsilon_2, \mu_2$ ) are the  $\epsilon$  and  $\mu$  of the particle's bulk material,  $\theta = ka\sqrt{\mu_2\epsilon_2}$  and  $k = 2\pi/\lambda$ . Note that  $\epsilon_p \neq \epsilon_2$  as it is the value the particle will have to possess to "produce the same electrical effect" [1].

From [4], the effective  $\epsilon$  and  $\mu$  is given by:

$$\epsilon_{eff} = 1 + \frac{N\alpha_1}{1 - N\alpha_1/3}, \quad \mu_{eff} = 1 + \frac{N\beta_1}{1 - N\beta_1/3} \quad (2)$$

where  $N$  is the number of particles per unit volume related to  $f$  by  $f = 4\pi Na^3/3$ ,  $\alpha_1 = \frac{6\pi i a_1}{k^3}$  and  $\beta_1 = \frac{6\pi i b_1}{k^3}$  are the particle's electric and magnetic polarisabilities, and  $a_1$  and  $b_1$  are the electric and magnetic scattering coefficients, given respectively, in general, as:

$$a_m = \frac{n\psi_m(nx)\psi'_m(x) - \psi_m(x)\psi'_m(nx)}{n\psi_m(nx)\xi'_m(x) - \xi_m(x)\psi'_m(nx)}$$

$$b_m = \frac{\psi_m(nx)\psi'_m(x) - n\psi_m(x)\psi'_m(nx)}{\psi_m(nx)\xi'_m(x) - n\xi_m(x)\psi'_m(nx)}$$

where the subscript  $m$  denotes different modes,  $n$  is the refractive index of the particle,  $\psi_m$  and  $\xi_m$  are the Riccati-Bessel functions [10].

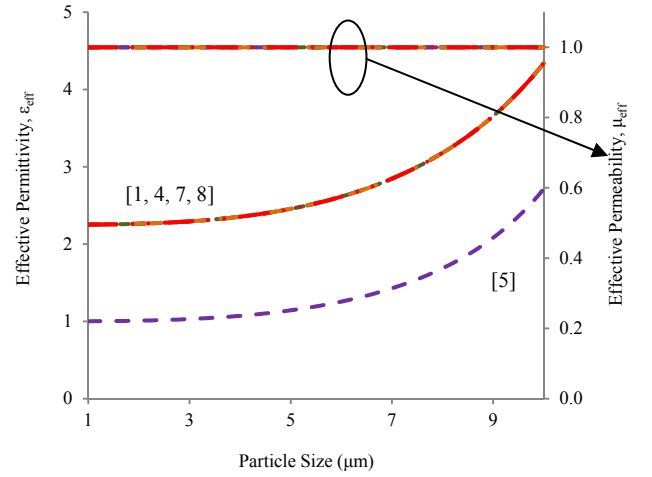
### III. PARAMETRIC STUDIES

To understand the response of the  $\epsilon_{eff}$  and  $\mu_{eff}$  of heterogeneous media to the different parameters constituting their canonical representations, each of these parameters was varied individually. They include: frequency, particle's size,  $a$ , and spacing,  $s$ , the particle's permittivity,  $\epsilon_2$  and permeability,  $\mu_2$  and the host's permittivity,  $\epsilon_1$  and permeability,  $\mu_1$ . Fig. 1

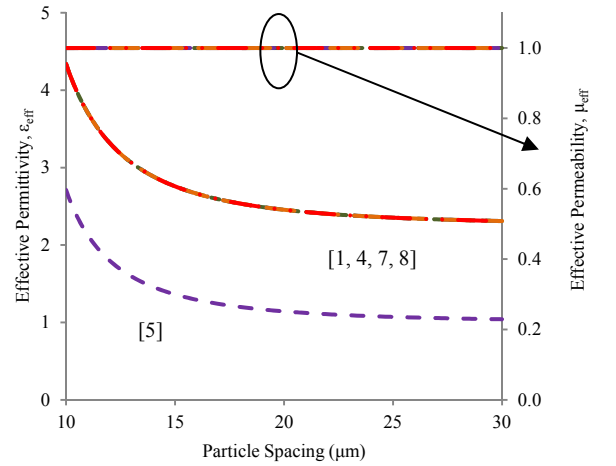
shows the effect of the particle's size and spacing and the frequency on the effective properties of the medium. The values used for each graph are given in Table 1. Other parameter values:  $\epsilon_2 = 7.8(1-j0.005)$  (Dupont),  $\mu_1 = \mu_2 = 1$ ,  $\epsilon_1 = 2.25(1+j0.001)$  (Polyethylene).

TABLE 1  
VALUES USED IN FIG. 1(A)–(C)

	$a$ ( $\mu\text{m}$ )	$s$ ( $\mu\text{m}$ )	Frequency GHz
Fig. 1a	1-10	20	1
Fig. 1b	5	10-30	1
Fig. 1c	10	25	1-50



(a)



(b)

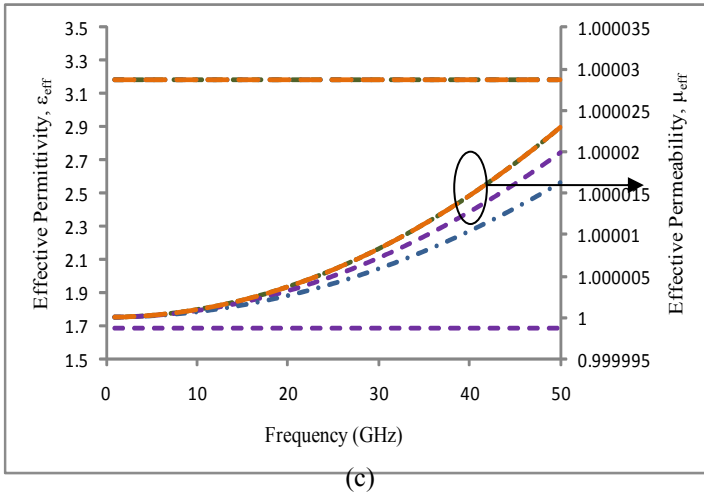


Fig. 1 Variation of  $\epsilon_{eff}$  and  $\mu_{eff}$  of a cubic lattice, heterogeneous mixture with (a) particle size,  $a$  (b) particle spacing,  $s$  and (c) frequency using the different analytic models in: [1] ( $\cdots$ ), [4] ( $-\cdot-$ ), [5] ( $---$ ), [7] ( $- \cdot -$ ), [8] ( $---$ )

The particle sizes in Fig. 1 were used as in some nanofabrication techniques (e.g. chemical deposition), nanoparticles are clustered together to form micro-sized objects. The results using [1, 4, 7, 8] show good agreement with each other and give confidence to applying their analytical representations for the effective  $\epsilon$  and  $\mu$  of heterogeneous media. Results from [5] differ as they do not include the permittivity of the host and should only be used when the host's permittivity and permeability approximate a vacuum. The  $\epsilon_{eff}$  can be controlled by varying  $a$ ,  $s$  and  $\epsilon_2$ . There's little variation in  $\mu_{eff}$  when  $\mu_1 = \mu_2 = 1$ .

#### IV. ELECTROMAGNETIC SIMULATIONS

The analytical results in Section III can be validated using EM simulations of these heterogeneous structures. Using a suitable EM simulation tool, such as the Finite Difference Time Domain (FDTD) EMPIRE XCcel™, the effective  $\epsilon$  and  $\mu$  of any structure can be retrieved using inverse scattering algorithms [11-14] on the Scattering (S-) parameter results obtained from the simulations. The formulation used in [11] was used in this paper. An EM plane wave was used as the excitation in which the Magnetic (H) and Electric (E) fields were polarised in the  $y$ - and  $z$ - directions respectively. As the canonical analyses assume semi-infinite structures, the microstrip line in EMPIRE was used for simulations with magnetic and electric boundaries in the  $y$ - and  $z$ - axes, making the model infinitely periodic in those directions. Absorbing boundaries were placed at either end of the microstrip line. Different numbers of layers of inclusions in the direction of propagation (along  $x$ -axis) were used (see Fig. 2).

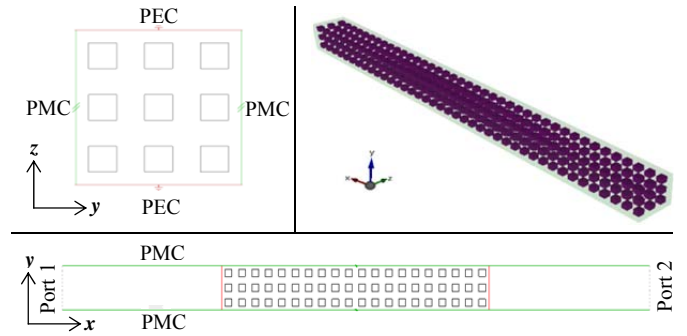


Fig. 2 Cross-sections of simulation domain and 3-D view of cubes in the homogeneous host medium

The resonant inverse scattering equations in [11] are a function of  $S_{11}$ ,  $S_{21}$ , sample thickness and frequency, from which the effective wave impedance,  $\eta$  and refractive index,  $n$  of the mixture can be derived. As the plane wave undergoes a phase change as it travels through the material, there is a discontinuity at certain frequencies, as there's an *arccos* function in its representation. As a continuous phase as a function of frequency is required for accurate results, this phase has to be subjected to a "rectification algorithm" that eliminates these discontinuities. The discontinuous and the rectified phases are shown in Fig. 3. A logarithmic scale is used on the  $y$ -axis to emphasize these discontinuities. Once the phase has been rectified,  $\eta$  and  $n$  can be calculated and then the  $\epsilon_{eff}$  and  $\mu_{eff}$  of the mixture, using  $\epsilon(\omega)$ ,  $\mu(\omega) = n(\omega)/\eta(\omega)$ ,  $n(\omega) \cdot \eta(\omega)$ , where  $\omega$  is angular frequency.

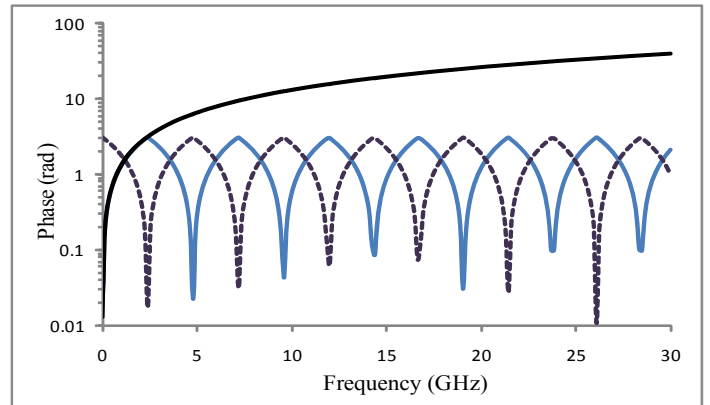


Fig. 3 Discontinuous phase  $\Delta\phi_d$  ( $-\cdot-$ ),  $\pi - \Delta\phi_d$  ( $---$ ) and rectified phase ( $---$ )

For further accuracy, the excitation and measurement planes, represented as 'Port 1' (or P1E) and 'Port 2' (or P2) in Fig. 2, should not touch the structure to avoid measuring higher order modes. The structure is excited at port 1. Thus, distances between the structure and these planes have to be accounted for as they represent the phase changes of the S-

parameters over those distances. This process is described below.

Let the distance from P1E to the start of the slab be  $d_1$ , and the distance from P2 to the end of the slab be  $d_2$ . Let the phase of the  $S_{11}$  obtained from the simulator be  $\varphi_1$  and the phase of the  $S_{21}$  be  $\varphi_2$ . The correct S-parameter phases,  $(\varphi_{1c}, \varphi_{2c})$  at the surface of the slab required for the inversion process are given by:

$$\varphi_{1c} = \varphi_1 + 2k_0d_1 \text{ for the } S_{11}, \text{ and}$$

$$\varphi_{2c} = \varphi_2 + k_0d_2 + k_0d_1 \text{ for the } S_{21}, \text{ where } k_0 = 2\pi/\lambda$$

As a first step, the inversion process was validated by reproducing the results in [11]. After this, a homogeneous slab of known permittivity was simulated for further validation. It is very challenging to simulate many micro-sized objects using FDTD as the memory requirements and runtimes become very large. Therefore, in order to validate the analytical equations with the EM simulations, larger objects were used. 0.5mm cubes spaced 1mm apart were used for quicker simulations and accurate meshing to avoid the stair-casing errors that spheres suffer from. Data used:  $\varepsilon_1 = 1.05(1+j1 \cdot 10^{-4})$ ,  $\varepsilon_2 = 44(1-j1.25 \cdot 10^{-4})$ ,  $\mu_1 = \mu_2 = 1$ , frequency range 1-30GHz.

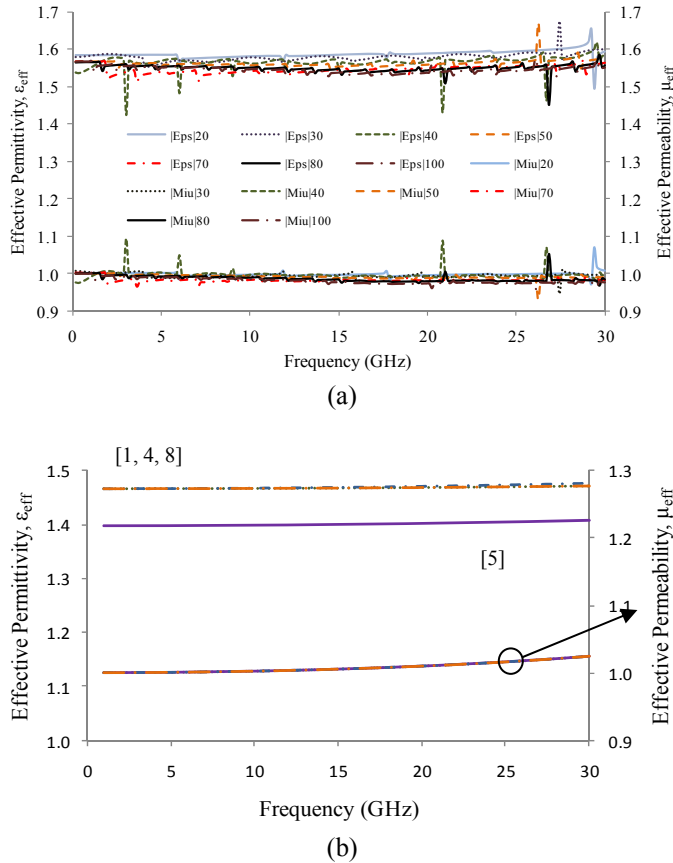


Fig. 4 Variation of  $\varepsilon_{eff}$  and  $\mu_{eff}$  of a cubic lattice, heterogeneous mixture with frequency from (a) simulations via inverse scattering equations for different layers of inclusions and (b) canonical analysis in [1] (.....), [4] (---), [5] (—), [8] (---)

The values in Fig. 4 are absolute values of the effective  $\varepsilon$  and  $\mu$ . The numbers in the legend in Fig 4 (a) signify the number of layers of inclusions along the x-axis in the FDTD simulation, for example |Eps|20 and |Miu|20 show the effective  $\varepsilon$  and  $\mu$  with 20 layers of cubes.

To obtain a canonical equivalent of the simulations with cubic inclusions, an equal volume process was used to find an equivalent value of sphere radius ( $a \approx 0.3102\text{mm}$ ) which would have the same volume as the cube. This radius value was then used in the analytical equations. As depicted in the graphs in Fig. 4 (b), the canonical equations give an average  $\varepsilon_{eff} = 1.47$ , while the FDTD simulations give an average  $\varepsilon_{eff} = 1.56$ , for all the layers examined. This difference in the values is due to cubes being used in the simulations, while in the canonical analysis spheres were used. Also, while the canonical equations assume semi-infinite structures, the simulation and inversion processes are limited in the number of layers of inclusions. Worthy of note is the fact that the effective values from the FDTD simulations generally tend to that of the canonical equations as the number of layers increased from 20 to 100 in the direction of propagation as shown in Fig. 5.

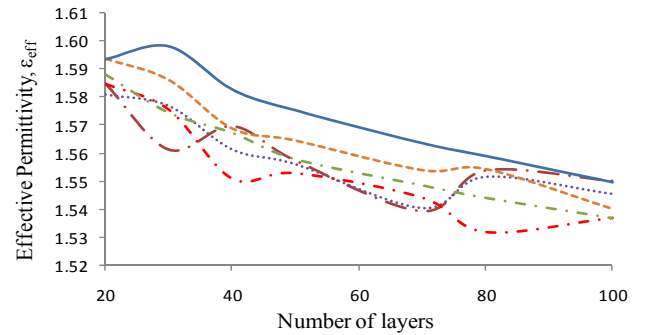


Fig. 5 Variation of  $\varepsilon_{eff}$  of a cubic lattice, heterogeneous mixture with number of layers of inclusions from simulations via inverse scattering equations for 5.1GHz (—), 10.05GHz (.....), 15GHz (---), 19.95GHz (— · —), 25.05GHz (— — —) and 30GHz (—)

Fig. 4(a) shows ‘spikes’ in the results which occur at the points where the plane wave experiences almost 100% transmission through the sample and so the  $S_{11}$  results are practically zero. Thus, they represent numerical errors from the simulation and inversion process and are not real phenomenon. These are spurious resonances and can be eliminated from the graphs by applying cut-off limits to the scattering parameters [11]. Fig. 4(b) reiterates the fact that the equations in [5] do not consider the permittivity and permeability of the host, and therefore the results differ from the equations from the other canonical models.

## V. CONCLUSIONS

In this paper, we show that the effective permittivity and permeability of a heterogeneous substrate obtained via analytical equations from the literature agree reasonably with

those obtained via resonant inverse scattering formulations using results from EM simulations. Note, cubical inclusions were used in the simulations for comparisons as a compromise between speed and accuracy. This work gives us confidence that the two separate techniques can be used to design and control the permittivity of heterogeneous substrates. With the rapid progress being made in nanomaterials fabrication techniques, this work facilitates new advantageous methods of advanced substrate and antenna manufacturing.

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