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Metallic Inclusions in a Non-Uniform Lattice

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Abstract— This paper is part of a larger project which aims to investigate the fabrication and electromagnetic advantages of creating integrated antenna systems using emerging nanomanufacturing technology. It has been known for several decades that the effective permittivity of a mixture consisting of dielectric inclusions in a host dielectric can be controlled by varying the permittivity, size and spacing of the inclusions. Various authors have developed theoretical equations to analyse these structures but are typically limited to spherical inclusions in a uniform cubic lattice. This paper extends this work from spheres in a uniform mesh to investigate thin metallic inclusions in a dielectric host using a non-uniform lattice (spacing in x, y and z, not the same). Electromagnetic simulations of these structures have been compared to canonical equations of spheres in a cubic uniform lattice with the same volume ratio.

I. INTRODUCTION

The creation of novel substrates with high permittivity values using low-cost materials will provide antenna and material engineers a variety of dielectric and magneto dielectric substrates that have the potential of being custom-made. These synthesized materials can be formed from homogenous materials within which are embedded inclusions of different sizes and in different lattice arrangements, typically cubic. The sizes and arrangement of these inclusions are dependent on the specific requirements. This potential to manipulate existing materials has prompted extensive research [1]-[11] into the creation of these materials that provide the electromagnetic (EM) properties, losses and other parameters required for the system to have. Related research has been in the areas of metamaterials [5], artificial materials [7] and double negative materials [9], [10]. Nano-technology fabrication techniques can be used in the creation of these heterogeneous structures [12]-[14], by using additive manufacturing processes as opposed to destructive processes, such as electrodeposition and self-assembly. Complete antenna structures and associated RF circuitry (as shown in Fig. 1) are possible by strategically placing metallic and insulating elements. The ability to control the particles’ volume ratio allows for the creation of novel and custom-made substrates. Faster build processes and reduced production costs are potential advantages of this nanofabrication method. Material cost reductions are expected to become significant as the world consumes more raw resources and this is particularly true as the average cost of dielectric materials increases with the increase in their permittivity values. In addition, EM advantages relative to bandwidth, size and efficiency, can be achieved by different methods.

In [15], we show what our intended antenna structure might be in the long run and not what has been achieved already. In the diagram, all the components of the antenna system are made from smaller particles.

The aim of this paper is to present our investigations of heterogeneous media with emphasis on their use as substrates in microwave designs. In Section II, we give a brief account of relevant equations from reviewed literature on the effective EM properties of infinite heterogeneous media. We also present a “resonant inverse scattering” method from [16] of extracting the $\varepsilon$ and $\mu$ of a material from the scattering (S-) parameters obtained from 3D Finite Difference Time Domain (FDTD) simulations using Empire XCell™. A detailed review was presented in [15], [17]. In Section III, an overview on the determination of the dielectric constants of metals such as Copper, using the Drude model [18], [19] is presented. A look at a uniform (that is, equal spacing in the x, y and z directions) and non-uniform (in only the x direction) heterogeneous structure having Copper inclusions is also presented. Conclusions are made in Section IV.

Small-sized dielectric inclusions having a higher permittivity and/or permeability can be added to a low dielectric, homogenous host to increase the effective electromagnetic (EM) properties of the final mixture. This has been proven both theoretically and via measurements. In our previous papers, we have reviewed such literatures and presented simulations for comparisons. In order to cause a significant increase in the effective permittivity of the mixture, metallic or conducting small-sized inclusions can also be added [1], [6], [20]-[22]. Note, that in this paper the permittivity and permeability values are the relative values and should be scaled by the free space values.
II. THEORETICAL AND EM SIMULATION ANALYSIS

The theories established in [1] form the general basis for the study of heterogeneous substrates/artificial dielectrics, although the earliest study is in [2]. The Clausius-Mossoti equation is used in [4]-[9] for describing the effective EM properties of a heterogeneous material. However, this equation is represented differently in the literature as: some exclude the EM properties of the host [5]; only examine the static DC case and have no frequency terms [7][8]; treat the particles’ densities and polarisabilities differently in electric and magnetic modes [9] or does not distinguish between the inclusion’s EM properties on a small or bulk scale [8]. They are similar in that their analyses are based on an infinite or semi-infinite medium. In general, an expression for the effective EM properties of a heterogeneous medium is given in [4] as

\[ K_{\text{eff}} = K_1 \left[ \frac{\left(K_2 + 2K_1\right)\left(K_1 - K_2\right)^{-1} - 2p + C(K_1, K_2, p)}{\left(K_2 + 2K_1\right)\left(K_1 - K_2\right)^{-1} + p + C(K_1, K_2, p)} \right] \] (1)

where \( K_1, K_2 \) and \( K_{\text{eff}} \) are the appropriate EM parameters of the host material, the inclusions and the mixture respectively; \( p \) is the volume fraction of the inclusions, which is based on the local unit cell of the medium. \( C(K_1, K_2, p) \) represents corrections for higher-order multipole terms as a result of the scattered fields [1], [23].

3D FDTD simulations have been used to simulate heterogeneous media to allow for finite and/or asymmetric structures. The effective \( \varepsilon \) and \( \mu \) of a medium can be obtained from the S-parameters as shown in [16], [24]-[26]. The S-parameters obtained were used in an Inversion process [16] to obtain the effective \( \varepsilon \) and \( \mu \) of the simulated structure. This also allows comparison with the results from the canonical analysis. The infinite medium assumption from the equations was replicated in the simulations with the use of Perfect Electric and Magnetic Conductor (PEC and PMC) boundaries on the two axes forming the plane of incidence of the plane wave impinging on the structure. The structure was finite along the axis of propagation.

In the equations and simulations, cubical lattices are used, that is, the inclusions are at the same distance from each other in all axes. Also, spherical inclusions are used in both.

A. Theoretical Results

Graphical results using [1], [5], [6], [9] are presented in Fig. 1 for dielectric inclusions. Data used: particle’s size, \( a = 50 \mu m \), particle size, \( s = 105 \mu m \), \( \varepsilon_2 = 10.21 \), \( \mu_1 = \mu_2 = 1 \), and \( \varepsilon_1 = 2.08 \).

Note, the equations in [5] do not include the host permittivity value and are accurate when the host is close to air but caution should be applied when using the equations in [5] to calculate effective permittivities where the host is greater than 1. Fig. 1 shows that the other equations from the literature agree over the frequency range considered. The average effective permittivity, \( \varepsilon_{\text{eff}} \) of the heterogeneous structure from the canonical equations is 4.23.

B. FDTD Results

To compare the theoretical equations with electromagnetic simulations, the heterogeneous sample was placed in a transmission line. By using magnetic and electric boundaries the samples are infinite in directions perpendicular to the transmission line while the sample is finite in the direction parallel to the transmission line. A rectification algorithm can be used to extract the effective permittivity from the simulated S11 and S21 results [17]. Using the same data as in section A, the effective \( \varepsilon \) and \( \mu \) of the structure is as shown in Fig. 2. The average \( \varepsilon_{\text{eff}} \) from the simulations is 4.4. This value compares very well with the values from the theoretical equations, and shows that the results from simulations and the inversion process can be used to acquire the effective EM properties of the heterogeneous medium.

The spikes shown in Fig. 2 at ~ 23 GHz reflect the measurement uncertainty in the extraction of the effective parameters due to the thickness resonance of the structure at that frequency.
III. METALLIC INCLUSIONS

The theoretical and FDTD processes have been extended to the case where the inclusions are metallic. In order to obtain an accurate comparison between theory and simulations, the Drude model was used to obtain the dielectric constant, $\varepsilon_r$, of a metal inclusion, in this Copper (Cu), see equation [19].

$$\varepsilon_r = \varepsilon_d - \frac{\omega_p^2}{(2\pi f)^2 + \omega_p^2}(1 + j \frac{\omega_p}{\pi f})$$

(2)

where $\omega_p = \frac{n_e e^2}{\varepsilon_0 m_e}$ is the plasma angular frequency, $\varepsilon_d$ is the dark dielectric constant, $\nu_p$ is the collision angular frequency, $m_e$ is the mass of the electron, $e$ is the electron charge, $\varepsilon_0$ is permittivity of free space, $f$ is frequency. In our calculations, $\varepsilon_d$ was chosen arbitrarily as its value is usually too small to have a significant effect on the second term of the equation. For Copper, $m_e = 1.3 m_0$, $m_0$ is free electron mass, $\nu_p = 4.23 \times 10^{13} s^{-1}$. Using (2) gave $\varepsilon_r = (1.27 - j103.53) \times 10^6$, at 10 GHz.

These values of permittivity allowed us use the canonical equations in instances where Copper particles were the inclusions. Due to this very high value of $\varepsilon_r$ (Copper inclusions), the theoretical maximum by which the effective permittivity of a host medium can be increased by is four times [1]. The effective permittivity of a heterogeneous medium with metallic inclusions is significantly dependent on the volume fraction of the inclusions.

A. Non-Uniform Lattice

In this section, thin metallic inclusions are placed in a non-uniform lattice. At the end of this section the results are compared to spheres in a cubic lattice with the same equivalent volume fraction.

Investigating non-uniform lattices will increase the range of applicable fabrication techniques. Given that spherical inclusions would be difficult to reproduce in the laboratory for initial measurements, the next stage in our research was to study the effective permittivity of Copper squares etched onto a readily-available dielectric such as GTS. GTS has a relative permittivity of 3 and a standard thickness of 125 μm. The thickness of the cuboids is 35 μm. The Cu ‘cuboids’ measure 500 μm x 500 μm x 35 μm, spaced 1000 μm apart in the Y and Z axes, and separated by the GTS thickness in the X axis. Thus the periodicity of the structure is 1000 μm in the Y and Z directions and 195 μm in the X direction. This geometry is based on sizes and materials that could be easily etched.

By stacking a number of layers together as shown in Fig. 3, we can understand how the total structure’s effective permittivity changes with the number of layers, and see if it matches the value from the canonical equations when an equivalent volume fraction is used to approximate a periodic structure.

The stacking gives the Cu a 70 μm thickness. Fig. 3 shows a 4-layer structure simulation set-up using the FDTD technique mentioned in Section II. The air gaps between the stacks has an effect on the value of the host permittivity, $\varepsilon_1$. As shown in Fig. 4, as the number of layers increase, the effective permittivity of the structure tends towards a certain value. The 12 and 14-layer values are significantly different from the 2-layer value. From previous work [16], we have found that thin samples do not produce the expected results and typically the accuracy of the simulations and the related effective permittivity extraction method increases with thicker samples.

From Fig. 4, as the number of layers increases, the effective permittivity of the dielectric/copper composition converges to an average value of 3.81. By using the volume of the Cu cuboids to find an equivalent sphere radius, and the Cu’s volume fraction to obtain approximate cubic lattice spacing, the stacked layer structure can be equated to spheres evenly spaced in a cubic lattice which in turn allows comparison with the theoretical equations. These calculations give an equivalent sphere radius of 161.06 μm and cubic spacing of 579.89 μm. The results from the equations which give an $\varepsilon_{eff}$ of 3.89. The results from the FDTD simulation of these sphere give an $\varepsilon_{eff}$ of 3.91 as shown in Fig. 5. These results indicate there is good agreement between the non-uniform stack using the FDTD method and the equivalent structure composed of spheres in a cubic uniform lattice using both the empirical equations and also the FDTD method.

![Fig. 3. (a) 2D and (b) 3D representation of a 4-layer stack of heterogeneous medium with 35 μm thick Cu etchings on 125 μm GTS substrate](image)
The canonical equations were found to agree well with EM simulations and the rectification algorithm when spheres were positioned in a uniform lattice. This geometry is reasonably well understood, however there is uncertainty as to the electromagnetic behavior when the inclusions are not spherical and are not evenly spaced. A structure consisting of metallic inclusions in a non-uniform lattice has been examined in this paper. The results showed good agreement with the equivalent volume fraction using spheres in a cubic uniform lattice. The results in this paper show that different inclusion geometries in non-uniform lattices will produce similar results and also that the inclusion permittivity and the volume filling ratio are the dominant parameters to determine the effective permittivity. These results indicate that we can design and fabricate our heterogeneous substrates using different geometries and that we can initially estimate the effective permittivity of a mixture by using the canonical equations. Note, higher effective permittivities can be produced using higher volume fractions of the inclusions. Future work will design geometries that will produce greater contrasts between the effect and the host permittivity and hence will facilitate comparison with measurements. Experimentally, it is possible to fabricate nanomaterials samples where the size of embedded inclusions can be varied from the nm range up to the level of mm, while their spatial arrangement can vary from a high degree of order to randomness.

REFERENCES


