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A UNIT CELL APPROACH TO MODEL AND CHARACTERIZE THE METAL POWDERS AND METAL-DIELECTRIC COMPOSITES AT MICROWAVE FREQUENCIES

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Abstract—A unit cell based numerical approach to model the metal powders and metal-dielectric composites at microwave frequencies is proposed. The unit cell based numerical modeling helps to compute the equivalent reflection and transmission coefficients of these materials, which are commonly used measured parameters at RF and microwave frequencies. The computation of the reflection and transmission coefficients of these artificial dielectric samples also facilitates the determination of their effective constitutive properties, defined in terms of the effective permittivity and permeability, using the reflection transmission approach. The applicability of the proposed unit cell method is first verified for some mixed dielectrics using the classical mixing formulas, and the standard waveguide approach. Once the validity of the proposed approach is ascertained, the effective constitutive properties of copper powder is determined. A detailed parametric analysis is also carried out in order to study the effect of various parameters such as the packing fraction, the grain size and the gap between adjacent spherical shaped metal particles, on the effective constitutive properties of the copper powder compact. This detailed analysis is quite helpful in order to optimize various parameters of the microwave sintering of metal powders and metal-dielectric composites before the actual start of the sintering process using microwaves.

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1. INTRODUCTION

The use of microwave technology for industrial material processing applications has been increasing in recent years due to certain advantages offered by the microwave heating such as the reduced cycle time, the volumetric and selective heating, the highly efficient processes and saving of energy etc. [1, 2]. The microwave energy has traditionally been used to heat lossy dielectrics such as food items for home appliances, and certain class of polymers and composites for various industrial applications [3–5]. However, recently, there has also been lot of interest to explore the use of microwave technology for sintering of metal powders after a study showing the absorption of microwaves by metal powders under certain conditions [6–8], and it has been reported that the microwave sintering could provide improved mechanical properties along with the finer micro structures [9] as compared to the conventional sintering. As the bulk metals reflect microwaves, hence the basis of microwave heating of metal powders can only be understood by realization of the basic fact that the metal powders should be treated as lossy dielectrics having mixtures of metal particles embedded in a host dielectric medium which may be considered as air for a very simple case. It is with this assumption that the effective medium theory has been used in the past to model the metal particles as a composite medium, where a dielectric oxide shell has also been introduced by many authors between the metal particles and the surrounding air medium [8, 10, 11]. The core-shell mixture model of these metal powders was mainly introduced to take into account the increased penetration depth of microwave energy inside these metal powder samples. However, apart from the core-shell model, the classical mixing formulas such as the Mean-field approach by Maxwell-Garnett [12], the Litchenker's Logarithmic mixture formula [13, 14], the Bruggeman mixing formula [15], the analytical approaches using the diagrammatic expansions [16] and Fourier series [17] have also the potential to be used for the metal powder composites in a way similar to the dielectric mixtures for which these formulas were originally proposed. A detailed study about the use of various classical and core-shell mixing formulas for the computation of effective permittivity of various metal composites has recently been presented in [18], where it is concluded that most of these formulas provide an error of the order of 10% when compared with some experimental data. However, the experimental data of the complex permittivity of the metal powders employed for comparison in [18] have mainly been obtained using the cavity perturbation technique [7], which is usually valid for low loss samples [19] as it is based on the assumption that the test

specimen does not change the field configuration significantly inside the cavity. It looks rather more appropriate to make use of the reflection-transmission approach [20, 21] instead of the cavity resonant technique to estimate the effective dielectric and magnetic properties of metal powders. The reflection-transmission approach is not based on any serious assumption, and has successfully been employed to measure the electromagnetic properties of the uniaxial composites [22] and the metamaterials [23–25] apart from the homogeneous materials in the microwave frequency band. In a general sense, the metal powders and the metal-dielectric composites may also be interpreted as metamaterials [26] since the electromagnetic properties of these powders and composites on a macro scale are quite different from its constituent materials. It is mainly due to this reason that the unit cell approach has been used here for the electromagnetic modeling and characterization of metal powders and the metal-dielectric composites. The unit cell based numerical modeling of metal dielectric composites is advantageous as compared to that of the classical mixture models and the shell-core models discussed above since the numerical model can take into account the minute details of the defined structure, and it is not also limited by the percolation limit usually applicable for classical models [27].

The aim of this paper is two fold. The first aim is to propose a unit cell based approach to model the metal powders and metal-dielectric composites at the frequency bands of 2.45 GHz and 30 GHz, which is achieved by defining appropriate unit cells for these types of artificial materials with the help of numerical full wave electromagnetic field simulators. The second objective of this paper is to estimate the effective constitutive properties of these metal powders and metal-dielectric composites using the reflection-transmission approach, which is facilitated here by defining the appropriate unit cells for these structures.

The numerical modeling of the mixed-dielectric and metal-dielectric composites is carried out by defining the unit cells having periodicity along the plane perpendicular to the direction of propagation. The basis of the unit cell models are the cubic bravais lattice structures widely used in the crystallography. The host material is a homogeneous cube with the spherical inclusion material arranged in the simple cubic (SC), the body centered cubic (BCC) and the face centered cubic (FCC) form. The unit cell based numerical simulations in the present case are performed using two standard electromagnetic field simulators, the CST Microwave Studio [28], and the Ansys HFSS [29] in order to obtain the scattering coefficients in the required frequency band. The CST Studio is based on the Finite

Integration Technique, and was recently used to model the copper powders at 2.45 GHz [30] using the unit cell concept in free space. The value of the dielectric loss reported by them for the copper particles having a packing density of 0.74 is, however, very low indicating a substantially low value of the effective conductivity which does not look appropriate from the practical point of view. In this paper, the general purpose frequency domain solver algorithm of the CST Studio is used to model the metal dielectric composites in the free space as well as in the waveguide environment at both 2.45 GHz and 30 GHz, which some times provides more efficient processing than at 2.45 GHz [8, 31]. The adaptive meshing technique of the CST Studio along with the S-parameter convergence criteria is used to generate the tetrahedral mesh of the defined structure, and accordingly the S-parameters are computed. In order to compare the results using various algorithms, the Ansys HFSS, which is based on the Finite Element Method, is also employed here. Its reliable classic mesh generates tetrahedral meshes at the desired solution frequency, and the field solutions are then obtained at the ports to extract the S-parameters of the structure using its frequency domain solver. For complex geometries involving wave guides with stacked unit cells, the HFSS is generally used in the present formulation.

The unit cell numerical modeling of the metal-dielectric and the mixed-dielectric composites basically provides the reflection and transmission coefficients at 2.45 GHz and 30 GHz in the free space as well as in the waveguide environment. The effective constitutive properties of these samples are then determined at both the frequencies in terms of the scattering coefficients using the standard method [24], which has been modified here for the waveguide dispersive media. To verify the proposed approach, firstly a number of mixed dielectric and simple composite media are considered in order to estimate the effective constitutive properties of these materials using the proposed unit cell approach. These estimated material properties are then compared with the standard Maxwell-Garnett law [12], the Logarithmic law of mixing [13, 14], and the Clausius-Mossotti relationship [32] for various volume fractions and permittivity values in order to validate the proposed approach. After this validation, the unit cells corresponding to the metal powders and metal-powder composites are defined to estimate their effective constitutive properties. In order to obtain the constitutive material properties using the waveguide approach, an array of $n \times m$ unit cells are employed to fill the cross-section of a WR-28 waveguide, and the effective values obtained using this approach are compared with the free-space unit cell approach at 30 GHz.

2. THE EFFECTIVE CONSTITUTIVE PROPERTIES AND THEIR ESTIMATION

The constitutive electromagnetic properties of the materials are usually defined in terms of the complex permittivity and permeability with its imaginary part mainly accountable for losses in the materials while the real part usually deciding the coupling of the microwave energy inside the test specimen. The complex permittivity of the test sample can be written as:

$$\epsilon^* \equiv \epsilon_0 \epsilon_r^* = \epsilon_0 \left[\epsilon_r' - j\epsilon_r''\right] = \epsilon_0 \left[\epsilon_r' - j\sigma_e/\omega\epsilon_0\right] \tag{1}$$

where the real and imaginary parts, ϵ_r' and ϵ_r'' are termed as the dielectric constant and the loss factor, respectively, ϵ_0 is the permittivity of free space, $\omega = 2\pi f$ is the radial frequency with f being the frequency in Hz, and σ_e is the effective electrical conductivity of the specimen taking into account both the dielectric and magnetic losses, which can also be defined as

$$\epsilon_r'' \equiv \frac{\sigma_e}{\omega\epsilon_0} \tag{2}$$

Similarly, the complex permeability of the test sample can be written as:

$$\mu^* \equiv \mu_0 \mu_r^* = \mu_0 \left[\mu_r' - j\mu_r''\right] \tag{3}$$

where again the real part μ_r' is usually defined as the relative permeability, and μ_r'' is termed the magnetic loss factor. At microwave frequencies, the permittivity and permeability of the test specimen can not be determined using any direct method. The usual procedure of finding these constitutive properties is to illuminate the test specimen with an electromagnetic wave of the desired frequency, and compute the ratio of the reflected wave and the transmitted wave to that of the incident wave widely known as the reflection (S_{11}) and transmission coefficients (S_{21}), respectively. It may be noted here that the reflection and transmission coefficients of the test specimen can be measured using a vector network analyzer by placing the sample either in free space or in a section of the rectangular waveguide. Hence, the main task in the estimation of constitutive properties of the test sample at RF and microwave frequencies requires the derivation of appropriate algorithms to obtain these properties in terms of the reflection and transmission coefficients. A number of techniques exist in the literature for this purpose as discussed earlier. In this paper, the technique presented in [24], which deals with the free space case assuming the plane wave or the TEM mode illumination, has mainly been used to obtain the constitutive properties of the unit cell in free space. For obtaining the constitutive properties of these

metal powder composites in the rectangular waveguide environment, which is also one of the objectives of this paper, the techniques presented earlier [22, 24] have been modified so as to make them applicable in the rectangular waveguide environment. The rectangular waveguide approach requires the precisely machined test specimen to be fitted inside the cross-section of the guide assuming the dominant TE_{10} mode illumination, which was earlier used to characterize nonmagnetic composite samples [22]. The propagation constant β of the test specimen placed inside the rectangular waveguide assuming the dominant TE_{10} mode illumination can be given by [33]:

$$\beta = k_0 \sqrt{\epsilon_r^* \mu_r^* - \left(\frac{c\pi}{p\omega}\right)^2} \tag{4}$$

where ϵ_r^*, μ_r^* are the complex relative permittivity and permeability of the test specimen, respectively, as defined earlier; $k_0 = \frac{\omega}{c}$ is the free space wave number with c being the velocity of light in free space; p represents the broader dimension of the rectangular waveguide. The impedance of the test specimen inside the waveguide for the dominant mode can be written as:

$$Z = \frac{\omega \mu_0 \mu_r^*}{\beta} \equiv \frac{\omega \mu_0 \mu_r^*}{k_0 \sqrt{\epsilon_r^* \mu_r^* - \left(\frac{c\pi}{p\omega}\right)^2}} \tag{5}$$

where, the value of β is substituted from (4). Meanwhile, it can be observed from (5) that

$$\frac{Z\beta}{\omega \mu_0} = \mu_r^* \tag{6}$$

From (6), it can be seen that if β and Z can be expressed in terms of the scattering coefficients, the value of μ_r^* can be calculated. Now, as explained in [22], the measured scattering coefficients of the test specimen at the sample interface can be defined in terms of the local reflection and transmission coefficients as

$$S_{11} = \frac{r_{local}\left(1 - t_{local}^2\right)}{\left(1 - r_{local}^2 t_{local}^2\right)} \tag{7a}$$

$$S_{21} = \frac{t_{local}\left(1 - r_{local}^2\right)}{\left(1 - r_{local}^2 t_{local}^2\right)} \tag{7b}$$

where, r_{local} is the *local* reflection coefficient defined at the sample interface, which can be written as

$$r_{local} = \frac{Z - Z_0}{Z + Z_0} = \frac{z - 1}{z + 1} \tag{8}$$

with $z = Z/Z_0$ as the normalized impedance, Z is the impedance of the test specimen inside the waveguide for the dominant mode given by (5), and

$$Z_0 = \frac{\omega\mu_0}{\sqrt{k_0^2 - (c\pi/p)^2}} \tag{9}$$

is the wave impedance of the air filled rectangular waveguide assuming the dominant TE_{10} mode propagation. The *local* transmission coefficient of the test specimen, t_{local}, in (7) is defined as

$$t_{local} = \exp(-j\beta d) \tag{10}$$

where d is the thickness of the test specimen, and β is defined using (4). Now, making use of (8) and after some algebraic manipulations, (7a) and (7b) can be solved to obtain

$$z = \pm\sqrt{\frac{(1+S_{11})^2 - S_{21}^2}{(1-S_{11})^2 - S_{21}^2}} \tag{11}$$

and

$$t_{local} = \frac{1 + S_{21}^2 - S_{11}^2 \pm \sqrt{\left(1 + S_{21}^2 - S_{11}^2\right) - 4S_{21}^2}}{2S_{21}} \tag{12}$$

The proper signs of z and t_{local} in (11) and (12) are chosen by applying the criterion that $|t_{local}| < 1$, and considering the fact that the test specimen of the effective metal-dielectric composite is always a passive medium [22, 24]. Now, once the value of t_{local} is obtained using (9), the value of β can be obtained using (10), and this value of computed β along with the value of z computed using (11) can be employed to determine the value of μ_r^* using (6). The value of ϵ_r^* of the test specimen can finally be calculated using (4) as the value of β and μ_r^* is already determined. It may be noted here that some times there may be some ambiguity in the solution of β using (10) due to multiple solutions, and under this situation some additional constraint has to be applied in order to select the correct solution [24].

3. NUMERICAL MODELING AND SIMULATION

The model considered in this paper to simulate the unit cell of the metal powders and composites is represented by a homogeneous cube of the host material or matrix with the inclusion of the spherical shape particles embedded into it. For simple metal powders, the host material may be taken as the air or the corresponding oxide medium with the inclusion as the metal particles of spherical shape. The host material

with the spherical inclusion is arranged in a simple cubic (SC), the body centered cubic (BCC), or the face centered cubic (FCC) form as shown in Fig. 1.

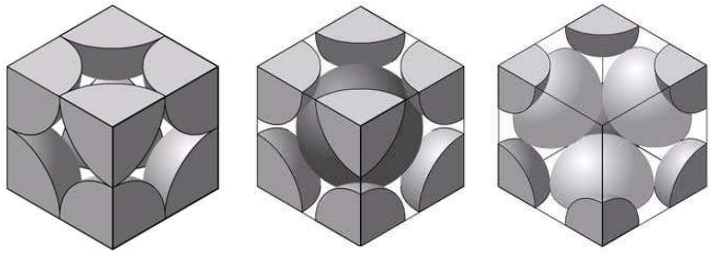

Figure 1. Figures (a) and (b) and (c) show the simple cubic (SC), body centered cubic (BCC) and face centered cubic (FCC) unit cells, respectively.

The typical model of a single FCC unit cell simulated using the 3-D electromagnetic field simulator ANSYS HFSS [29] is shown in Fig. 2, which basically consists of a dielectric or air cube (host matrix) of thickness a with the metallic inclusion of spherical shape having a packing fraction $p = 0.74$. The thickness a of the cube would depend on the incident wavelength, and the packing fraction mainly decides the effective constitutive properties of the artificial material simulating the metal-dielectric composite in the present situation. The unit cell lattice is considered to be infinite along the transverse y and z directions. For this, the PEC (perfect electric conductor) boundary condition is assigned to the upper and lower surfaces of the cube on the xy faces, and the PMC (perfect magnetic conductor) condition is applied along the side walls of the zx faces of Fig. 2, which also ensures a TEM mode propagation along the direction x with the orientation of the electric field along the z axis as shown in this figure. The whole geometry is then excited by two waveguide ports to compute the reflection and transmission coefficients over the specified frequency band at the pre-defined reference planes. The computational complexity of the structure is reduced by considering xy and zx as the electric and the magnetic symmetry planes, respectively, due to the constraints discussed above, which basically then requires only one quarter of the structure to be computed.

The numerical simulations were carried out for spherical particles in different lattice structures, i.e., SC, BCC, and FCC using the two electromagnetic field simulators, the HFSS and the CST Microwave Studio [28]. The adaptive meshing considering the tetrahedral mesh

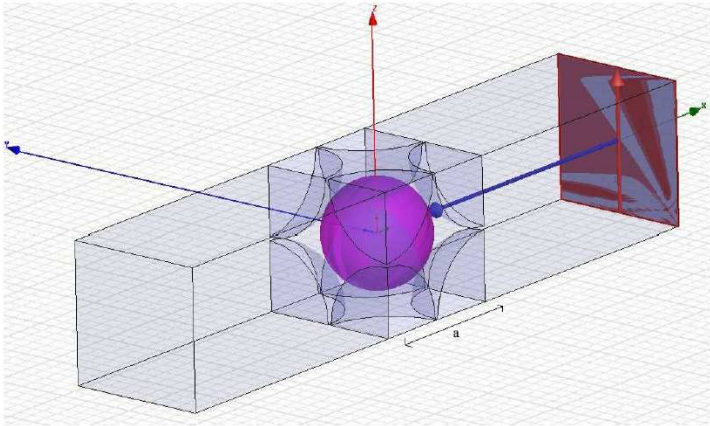

Figure 2. The unit cell model along with the excitation simulated in HFSS, a represents the thickness of the cube.

was employed to obtain a stable convergence of the desired solution. The diameter of the metallic spherical particles are taken to be in the range of 10–700 µm while the distance between neighbouring particles is varied between 10 nm to 10 µm. It may be mentioned here that the volume faction of the unit cell would depend upon the particle size as well as on the gap between these particles, and hence these two parameters can not be arbitrarily chosen. In this paper, the frequency domain solver of the simulator was employed to obtain the scattering parameters of all the considered structure at both 2.45 GHz and 30 GHz. The obtained scattering parameters, defined in terms of the reflection and transmission coefficients, S_{11} and S_{21}, respectively, are then used for the extraction of effective constitutive properties of the metal powders and metal dielectric composite using the procedure described above. It is to be noted here that under real world situations, the shape of the particles might be some times non-spherical due to various factors such as clogging of closely spaced particles especially during the curing process. However, in this paper, only the spherical particles are considered due to simulation constraints.

4. RESULTS AND DISCUSSION

The technique of numerical modeling and constitutive parameter extraction discussed in previous sections is applied here to analyze a number of mixed dielectric and composite materials having various unit cell structures. These materials are modeled using the proposed unit

cell approach, and accordingly the effective constitutive parameters of these materials are retrieved using the method discussed in Section 2. Firstly, the proposed unit cell approach is validated for some standard mixed dielectric samples by comparing the results of the proposed unit cell approach assuming a TEM mode propagation with those obtained by the conventional mixing formulas such as the *Maxwell-Garnett*, *Logarithmic laws* etc. Similarly, for metal-dielectric composites, the results from the *Clausius-Mossotti* expressions are compared with the proposed unit cell approach. Secondly, the unit cell model assuming the *TEM* mode propagation is compared with the conventional rectangular waveguide approach assuming the dominant TE_{10} mode propagation, and the effective constitutive properties obtained in both cases are compared. Finally, the proposed unit cell model is applied to the case of metal powders and metal dielectric composites, and the factors influencing its effective permittivity and permeability are evaluated.

4.1. Validation of the Unit Cell Approach with Various Mixing Formulas

The effective complex permittivity obtained using the unit cell approach is first compared with the conventional mixing formulas discussed earlier. Table 1 shows a comparison of the the complex relative permittivity obtained by the *Maxwell-Garnett Law*, *the Logarithmic Law*, and the proposed unit cell approach. The various lattices in this table represent different volume fractions, viz., SC = 0.52, BCC = 0.63, and FCC = 0.74, and the unit cell structure similar to that shown in Fig. 2 is modeled using the ANSYS HFSS software. The spherical particles of radius 100 μm are considered as inclusion in this case with no spacing between the individual particles in order to obtain the required volume fractions. The mixing laws usually consider two factors to calculate the effective permittivity of the composite mixture, viz., the permittivity of the inclusion and the host medium, and the volume fraction of the inclusion in the host medium. The unit cell approach, on the other hand, first models the appropriately defined unit cells of the composite material using the numerical electromagnetic filed simulator in order to compute the scattering coefficients of these materials, and then the effective constitutive properties of the material under test are determined from the scattering coefficients using the earlier described approach.

It can be clearly observed from Table 1 that both the real and the imaginary parts of the effective permittivity computed using the proposed unit cell approach match quite well with both the mixing laws given in this table. It can, therefore, be concluded that the unit cell

Table 1. Comparison of the effective complex permittivity using the mixing formulas and the unit cell approach at 30 GHz.

Lattice	Effective Relative Permittivity, ϵ_r^*		
	Maxwell-Garnett Law	Logarithmic Law	Unit Cell Approach
CASE 1: FR-4 Epoxy (inclusion) in air (host)			
SC	$2.156 - 0.019i$	$2.172 - 0.022i$	$2.571 - 0.025i$
BCC	$2.697 - 0.032i$	$2.739 - 0.037i$	$2.822 - 0.035i$
FCC	$2.943 - 0.038i$	$2.943 - 0.044i$	$2.935 - 0.041i$
CASE 2: Taconic RF-35 (inclusion) in air (host)			
SC	$1.937 - 0.002i$	$1.927 - 0.002i$	$2.233 - 0.002i$
BCC	$2.342 - 0.003i$	$2.344 - 0.003i$	$2.405 - 0.002i$
FCC	$2.520 - 0.003i$	$2.527 - 0.003i$	$2.484 - 0.003i$
CASE 3: Taconic CER-10 (inclusion) in air (host)			
SC	$2.939 - 0.003i$	$3.339 - 0.006i$	$4.159 - 0.005i$
BCC	$4.122 - 0.006i$	$4.786 - 0.011i$	$4.652 - 0.008i$
FCC	$4.742 - 0.008i$	$5.495 - 0.014i$	$4.953 - 0.009i$

approach provides results which are similar to classical mixing models in case of simple mixed dielectrics and composites, which also validates the applicability of the proposed unit cell approach. This is especially advantageous in case of metal powders and metal dielectric composites having higher values of the packing density where the classical mixing formulas fail because of their finite percolation limit.

In order to verify the proposed unit cell model for the case of metal-dielectric composites, the PEC is used as an inclusion in the air host medium. The classical *Clausius-Mossotti* expression used in [32] to analytically calculate the effective real permittivity of PEC spheres is employed for the validation in this case. The SC, BCC and FCC structures with same volume fractions as in Table 1, i.e., SC = 0.52, BCC = 0.63, and FCC = 0.74 are also used here. It may be noted here that the Clausius-Mossotti expression also takes into account the spatial arrangement of different constituents of the composite apart from their permittivities and the volume fractions. Table 2 compares the theoretical results of the *Clausius-Mossotti* equation with the values obtained using the proposed unit cell approach. The unit cell approach in this case uses spherical particles of radius 100 µm with the gaps between these particles adjusted to 7 µm.

Table 2. Permittivity values computed using the unit cell approach and the *Clausius-Mossotti* equation at 30 GHz.

Lattice	Effective Relative Permittivity, ϵ_r^*	
	Unit Cell Approach	Clausius-Mossotti Equation
SC	$6.01 - 0.03i$	5.891
BCC	$8.79 - 0.04i$	9.023
FCC	$9.96 - 0.07i$	10.925

It can be observed from Table 2 that for all the three types of lattice structures, the value of the real part of the effective permittivity estimated using the proposed unit cell approach matches quite well with that of the *Clausius-Mossotti* expression thereby validating the proposed approach for the metal-dielectric composites. It may be mentioned here that the *Clausius-Mossotti* expression provides only the real values of the complex permittivity, and hence only the real permittivity can be compared in the present case as shown in the third column of the above table.

4.2. Comparison of the Unit Cell Free Space Approach with the Waveguide Approach

The rectangular waveguide approach is one of the most widely used techniques to estimate the constitutive properties of materials at RF and microwave frequencies because of many practical advantages such as the preparation of the sample, availability of the accurate calibration standards etc. [22]. Hence, in order to make any constitutive propertied reconstruction technique practically viable in the microwave frequency range, the proposed technique should conform to the waveguide method. Another advantage of using the waveguide based technique as compared to the single unit cell based approach being used in the past [30], is that a number of unit cells are required in this case to fill the cross-section of the rectangular waveguide, which basically helps to know whether the unit cell defined under the particular situation is appropriate under the macro approximation simulating the real material. Under the ideal situation, the constitutive effective properties of the material extracted from the single unit cell using the *TEM* mode illumination should match with the properties obtained from the rectangular waveguide approach having the TE_{10} mode illumination. It is mainly due to the aforementioned reasons that the constitutive properties of a number of composite samples have been extracted using both the unit cell and the waveguide approach in this

paper, and accordingly the values obtained using both the approaches are also compared. For using the waveguide approach, a section of WR-28 waveguide is employed, whose cross-sectional dimensions are 7.11×3.56 mm with its operating frequency range as 26–40 GHz. As the waveguide approach requires the test specimen to completely fill its cross section, the dimensions of the unit cells are accordingly chosen. The unit cell lattices arranged in SC, BCC and FCC are used to compare both the approaches using appropriate retrieval methods described in Section 2. The typical unit cell model of the BCC lattice used in the present situation is already shown in Fig. 2, while the waveguide model corresponding to this unit cell is shown in Fig. 3 where a number of unit cells are stacked together in order to completely fill the waveguide cross section. The dimension of the unit cell is chosen as a compromise between the desired accuracy and the required processing time. In the present situation, the dimensions of the unit cell are selected to be $a = 1.78$ mm, and so 4×2 array of the unit cells is required to fit the cross section of the rectangular waveguide. The simulation of both the unit cell, and the waveguide structure filled with the required number of unit cells is carried out at 30 GHz. The main difference between modeling the single unit cell, and modeling a section of the rectangular waveguide filled with a number of unit cells can be summarized as follows:

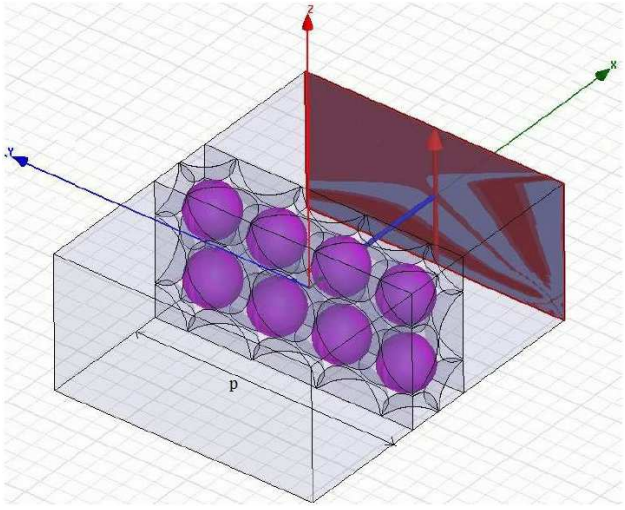

Figure 3. The waveguide model showing a number of unit cells fitted along its cross-section simulated using ANSYS HFSS, p represents the broader dimension of the designated waveguide.

(i) The free space environment is used for the unit cell approach, while a number of unit cells are stacked inside the section of a rectangular waveguide for the waveguide approach.

(ii) The unit cell approach uses a plane wave or the *TEM* mode excitation, whereas the waveguide approach makes use of the dominant TE_{10} mode illumination.

(iii) The *unit cell* boundary condition along the transverse dimensions is used to emulate the infinitely repeated cell structure in free space. However, for the rectangular waveguide, the perfect electric (*PEC*) boundary condition is employed along the transverse plane to account for the metallic walls.

(iv) The reference impedance value for the free space approach employing a single unit cell is the free space impedance of 377 Ω, while for the rectangular waveguide approach the wave impedance of TE_{10} mode is used as the reference value.

4.2.1. Comparison for Mixed-dielectrics

First of all, the mixed dielectrics are considered in order to compare the unit cell approach with the standard waveguide method. For this purpose, the dielectric spheres made of Taconic RF-35 ($\epsilon_r = 3.5$, $\tan\delta = 0.018$) are modeled with varying packing fractions (SC = 0.52, BCC = 0.63, and FCC = 0.74) using air as the host medium for all the three cubic structures in order to find out the scattering coefficients at the specified frequency in each case. The radius of the particles in this case are taken as 0.31 mm with no gap between them. Table 3 shows the effective permittivity and permeability values extracted from the scattering parameters for both the methods. It can be observed from this table that the effective constitutive properties obtained using both

Table 3. The extracted constitutive parameters for different lattices using the unit cell and the waveguide method (for mixed-dielectrics) at 30 GHz.

Method	Lattice	ϵ_r^*	μ_r^*
Waveguide	SC	$1.96 - 0.004i$	$0.90 - 0.0005i$
Unit Cell	SC	$1.85 - 0.007i$	$1.00 - 0.0002i$
Waveguide	BCC	$2.22 - 0.002i$	$0.88 - 0.0004i$
Unit Cell	BCC	$2.30 - 0.002i$	$0.98 - 0.0002i$
Waveguide	FCC	$2.22 - 0.002i$	$0.91 - 0.0015i$
Unit Cell	FCC	$2.48 - 0.003i$	$0.95 - 0.0007i$

the methods correlate to a good extent, thus verifying the proposed unit cell approach for the case of Mixed-Dielectrics. It is also to be noted that the scattering parameters for the unit cell approach and the waveguide method would not be same since they are defined with reference to different impedance levels for both the media as explained in the previous section. However, the effective constitutive properties obtained using both the methods should be similar because of the fact that the proposed estimation algorithm takes note of this change in reference impedance levels for the two media.

4.2.2. Comparison for Metal-dielectric Composites

After comparing the unit cell approach with the waveguide method for the mixed-dielectrics, the metal-dielectric composites, akin to the metal powders (copper spherical particles in the host medium), are considered. The host medium for simulating the Cu metal compact is taken as the Cu oxide rather than air, which provides the numerical stability and is also close to the real situation [7]. The relative permittivity of Cu oxide is taken as $\epsilon_r' = 9.483$ and $\epsilon_r'' = 0.0755$ at 30 GHz [30]. The unit cell structure for this case is defined using the particle size of diameter 0.62 mm, and the gap between the particles is taken as 0.01 mm for a faster convergence. Although the size of the particles considered here is quite large, but the main aim here is to compare the results of the unit cell approach with the waveguide method, and hence the relative values of these properties are more important. The packing fractions for the three lattices in the above structure are computed as SC = 0.495, BCC = 0.60, and FCC = 0.70. The simulation using the unit cell in free space and the unit cells arranged inside a section of WR-28 waveguide is carried out at 30 GHz using the conditions described earlier. The effective permittivity and permeability results for this case are given in Table 4. It may be noted from Table 4 that both the real and the imaginary parts of the effective complex permittivity increase gradually from the first two rows (SC) with the maximum value obtained for the last two rows (FCC). The reason for this change is that the packing density of the FCC case is maximum (0.74), which basically means the higher ratio of metal particles in the matrix thereby increasing the effective constitutive properties. It is to be clearly observed from this table that the values of the effective permittivity and permeability for both the unit cell approach and the standard waveguide method match quite well for all the cases thus showing the validity of the proposed approach in case of metal-dielectric composites and metal powders.

Table 4. The extracted constitutive properties for different lattices using the unit cell and the waveguide method (for metal-dielectric composites) at 30 GHz.

Method	Lattice	ϵ_r^*	μ_r^*
Waveguide	SC	$6.936 - 0.109i$	$0.754 - 0.120i$
Unit Cell	SC	$4.575 - 0.138i$	$0.796 - 0.019i$
Waveguide	BCC	$41.339 - 0.249i$	$0.989 - 0.003i$
Unit Cell	BCC	$50.000 - 0.202i$	$1.060 - 0.005i$
Waveguide	FCC	$58.346 - 0.070i$	$0.879 - 0.002i$
Unit Cell	FCC	$57.435 - 0.314i$	$0.920 - 0.004i$

4.3. Effective Constitutive Properties of Metal Powder Compacts and Their Dependence upon Various Parameters

Once the validity of the proposed unit cell model is ascertained for mixed dielectrics as well as metal-dielectric composites (metal powders), the unit cell model of the metal powder compact is studied in detail, which is also one of the main objectives of this paper. The copper particles of spherical shapes embedded in the copper oxide as the host medium with varying gaps between particles are considered for the analysis here. The modeling of the copper particles embedded in the oxide medium is done by considering them as the composite media, and accordingly an appropriate unit cell is defined to compute the scattering coefficients as discussed earlier. The effective constitutive properties of these metal powders are then extracted from the scattering coefficients using the proposed approach, which actually helps in controlling various parameters during the microwave sintering of metal powder compacts without resorting to the actual material processing. The information on the constituent properties of the metal powder compact also provides an idea about the coupling of the incident microwave energy with the test specimen as well as the extent of heating of the sample under the influence of microwaves.

The modeling of the actual copper powder compacts is done here by considering the FCC unit cell, which is basically the most closely packed cubic lattice for uniformly sized spherical particles. The modeling helps in studying the effects of various parameters such as the grain size, the packing fraction, and the gap between neighbouring metal particles, on the effective constitutive properties of the copper powders at both 2.45 GHz and 30 GHz, which are the two most commonly used frequencies for the microwave sintering of the metal powder compact. A close analysis of the effects of these

parameters on the effective permittivity and permeability of the metal powder compact is carried out using the numerical simulator, and is very helpful to understand the microwave sintering process as the constitutive properties of these materials quite significantly affect the overall sintering process using microwaves.

4.3.1. Effect of Grain Size

The metal powders usually come in various grain sizes, and it is expected that the size of the grain significantly affects the overall sintering behavior of these powders under the influence of microwaves for a constant packing density. For studying this kind of behavior, the radius of the copper powders is varied over a large value by keeping the packing density to be constant at 0.74 with the distance between the particles to be fixed at 0.01 µm, and its effect on the constitutive properties of the compact for two different sintering frequencies, i.e., 2.45 GHz and 30 GHz is calculated as shown in Table 5. This table basically represents the properties of Cu particles, and hence only the effective complex permittivity and the conductivity is computed as the effect on permeability would not be significant because of the nonmagnetic nature of Cu. From Table 5, the following observations can be made:

(i) The effective permittivity decreases with increasing grain size.

(ii) The value of effective permittivity is less at higher frequencies (30 GHz).

(iii) The value of the effective conductivity reduces drastically with the grain size. At 30 GHz, the conductivity is about 1.2×10^5 S/m for the particle size of 40 µm, whereas at 330 µm it gets reduced to 72 S/m.

Table 5. Effect of the grain size on the effective complex permittivity for Cu particles.

Particle size (µm)	ϵ_r^*	
	2.45 GHz	30 GHz
19.5	$992446.5 - 617876.3i$	$184939.0 - 62279.2i$
38.9	$416846.4 - 191464.0i$	$59579.5 - 12299.9i$
58.4	$231585.5 - 85937.8i$	$28855.3 - 4475.9i$
194.5	$31762.9 - 4947.1i$	$2759.8 - 176.2i$
213.9	$26937.3 - 3978.1i$	$2256.5 - 141.1i$
291.7	$15067.4 - 1704.0i$	$1099.6 - 77.6i$
330.7	$12229.3 - 1277.9i$	$797.7 - 72.1i$

It can be observed from the above table that the effective constitutive properties of the Cu powder is significantly high, which would result in much lower penetration depth of microwaves thereby not allowing the effect of volumetric heating [3] for these powders. Hence, the presence of significant thickness of native oxide layer between the metal particle looks more appropriate, which actually increases the penetration of these the microwaves inside the sample thereby enhancing the overall microwave heating inside the sample [7, 8]. It may be noted here that the value of the effective material properties given in Table 5 is quite large as compared to that reported in [30]. However, the effective constitutive properties data presented here look more sensible as at the 74% of the packing density, the equivalent material is expected to behave much like the bulk metal with the effective value of the loss factor given by (2), which in usual circumstances can not be very small unless a native oxide layer having a significant thickness is present between the metal particles as shown in the later part of this text.

4.3.2. Effect of Packing Fraction

In this study, the packing fraction of the FCC lattice is varied from 2% to 74%. This is done by keeping the unit cell size constant at 0.3 mm and varying the radius of the spheres within the cell to get the required packing fraction. The radius of the spheres is varied from 0.031 mm to 0.106 mm for a fixed unit cell size of 0.3 mm to obtain the required packing fraction. The unit cell size in the present situation is kept constant for various particle sizes by adjusting the gap between the particles in the range of 0.01 μm to 0.1975 mm, which basically changes the volume fraction of the inclusion in the host medium. Fig. 4 shows copper particles arranged in FCC with the limting packing fraction of 74%. The actual values of the constitutive properties for the Cu powder compact having the FCC lattice are shown in Fig. 5, where it can be seen that the increased packing fraction results into higher value of the effective permittivity and conductivity of the system. This kind of behavior is also anticipated as the increase in the packing density actually increases the fraction of Cu metal particles having much higher value of the conductivity as compared to the oxide host medium. Now, one of the important parameters responsible for the efficient microwave heating of a test specimen is the penetration depth, which actually decides the coupling of microwaves inside the material under test. The penetration depth quite strongly depends upon the effective constitutive properties of the test specimen, and hence once these properties are determined, the penetration depth of the test

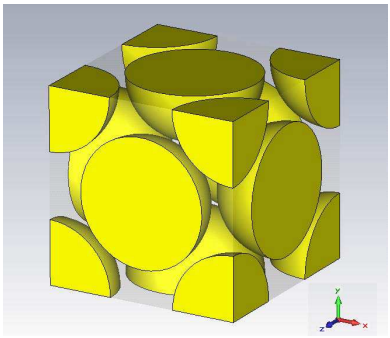

Figure 4. Copper particles arranged in FCC lattice at 70% volume fraction.

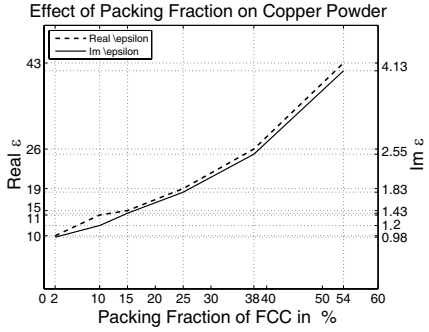

Figure 5. Variation in effective relative permittivity with packing fraction in FCC copper lattice at 30 GHz, at 74% $\epsilon_r^* = 7742.441 - 689.291i$.

material can be computed using the following expression [3]

$$D_p = \frac{1}{2\omega}\sqrt{\left(\frac{2}{\mu'\epsilon'}\right)}\left[\sqrt{\left(1+\left(\frac{\epsilon''_{eff}}{\epsilon'}\right)^2\right)}-1\right]^{-1/2} \tag{13}$$

where $\omega = 2\pi f$ is the radial frequency with f being the frequency in Hz. Table 6 shows the penetration depth of samples having various packing fractions considered here at both 2.45 GHz and 30 GHz. It can be observed that for a given packing density, the frequency of 2.45 GHz offers better penetration of microwaves and evidently more coupling as compared to that of 30 GHz, which is obvious from (13). It is, however, very important to note that for higher packing fraction, the penetration depth is significantly reduced, which would actually then not allow the microwaves to efficiently couple with the test material. Hence, the microwave heating of the metal powder compact for very high packing density is usually not feasible as per the present model unless a native oxide layer of significant thickness is introduced between various metal particles.

4.3.3. Effect of Gap between Copper Particles

It is obvious from the above discussion that the numerical model of the metal powders used to calculate the penetration depth is significantly affected by the introduction of the native oxide layer. Hence, it looks more appropriate to insert some native oxide layer between the metal

Table 6. Penetration depth for different packing fractions at 2.45 GHz and 30 GHz.

Packing Fraction (%)	Particle Size (μm)	Penetration Depth m	
		2.45 GHz	30 GHz
2	60	0.064	0.0053
4.6	84	0.063	0.0051
9.07	106	0.061	0.0050
15	126	0.058	0.0048
25	148	0.056	0.0045
37.7	170	0.053	0.0043
53.8	190	0.049	0.0040

Table 7. Effect of gap between copper particles.

Gap (μm)	effective permittivity ϵ_r^*	σ_r^* (S/m)	penetration depth m
0.010	$7842.13 - 697.22i$	1163.09	6.50×10^{-4}
0.032	$7836.00 - 692.41i$	1155.07	6.54×10^{-4}
0.055	$7699.71 - 672.14i$	1121.25	6.61×10^{-4}
0.077	$148.01 - 14.45i$	24.11	2.89×10^{-3}
0.100	$158.32 - 15.21i$	25.36	3.10×10^{-3}
1.000	$120.47 - 11.75i$	19.03	3.32×10^{-3}

particles to model the metal powder compact using the proposed numerical unit cell approach, as has been done earlier using the classical models [7]. It is mainly due to this reason that the gap between neighbouring copper particles is varied from 10 nm to 1 μm in this section by keeping the radius of the particle to be constant at 0.1 mm, which is akin to the presence of a varying oxide layer between particles, to model the effects of these changes. The FCC lattice with a packing density of 0.74, and the particle size of 0.2 mm has been considered for all these computations. The change in effective permittivity and penetration depth with the varying oxide layer thickness between the particles is shown in Table 7. It can be observed from Table 7 that increasing the thickness of the oxide layer between the particles, akin to the introduction of more gap between them, has a very significant

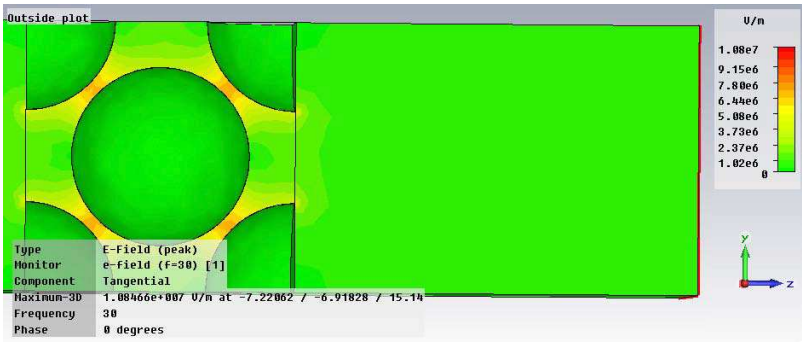

Figure 6. Electric field in the gap region of copper particles at size = 115 µm.

effect on the constitutive properties of the resultant metal powders. This kind of effect has also been reported earlier [7, 8], and can be attributed to the intense electric field developed in the gap region as seen in Fig. 6. The electric field in the gap region varies from 1.26×10^4 V/m to 4.07×10^7 V/m as the gap reduces from 1 µm to 10 nm. This increase in the effective constitutive properties with the reduced gap explains the neck formation between adjacent particles in the pre-sintering phase. It is known that the electric field does not penetrate copper beyond its skin depth but is squeezed between the gaps in powdered compacts eventually heating the gap region, leading to neck formation. Repeated exposure to the electric and magnetic fields strengthens the neck connecting adjacent particles with sharp rise in permittivity and conductivity, until the particles are completely sintered. The constitutive properties calculated by the unit cell model support the neck formation theory. It is also to be noted that increasing the thickness of the oxide layer between the particles increases the penetration depth of microwaves inside the metal powder compact, thereby explaining the microwave heating of metal powders having even higher values of the packing density.

5. CONCLUSION

A unit cell based numerical method has been presented to model the metal powder compact and the metal-dielectric composites. The constitutive properties of these metal powders have been determined using the reflection-transmission method, where the scattering coefficients values computed using the numerical method have been employed. The proposed approach has first been verified

using the standard mixing laws, and the Clausius-Mossotti expression. The applicability of the proposed unit cell has also been tested using the conventional rectangular waveguide approach, where a close match between the free space unit cell approach and the waveguide method shows the usefulness of the proposed unit cell based method for spherical shaped inclusion in the host medium. The effects of both micro level properties such as the arrangement of inclusion particles, the size of particles, the gap between neighbouring particles etc., as well as the macro parameters such as the volume fraction, the material properties of its constituents etc., on the effective constitutive properties of the resultant metal-dielectric composite have been studied. The effective constitutive properties of copper powders have been determined at frequencies of 2.45 GHz and 30 GHz, the two most commonly used frequencies used for the microwave sintering. It is found that the basic parameters such as the penetration depth, the dielectric loss etc., are different at two frequencies. It has also been observed that the presence of even a very thin native oxide layer between the copper metal particles has a very significant effect on the effective constitutive properties of the corresponding metal powder compact thereby verifying the earlier proposed effective medium theory for these metal-dielectric composites. However, the advantage of the present unit cell based numerical method is that lattices of any arbitrary structure can be modeled, and it also facilitates the use of standard free space and waveguide based reflection transmission approach to compute the constitutive properties of these metal powders and metal-dielectric composites.

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