Combined Numerical and Analytic Approach for Generalized Models of Complex Bi-Anisotropic Materials

Seung-Woo Lee, Akira Ishimaru, Yasuo Kuga, and Vikram Jandhyala

Department of Electrical Engineering

University of Washington, Seattle, WA 98195-2500 USA

ABSTRACT

A combined numerical and analytic approach is presented to obtain a general matrix form of constitutive relations for a bi-anisotropic material which consists of arbitrary inclusions in a host medium. This approach is based on the quasi-static Lorentz-Lorenz theory which relates the constitutive parameters of the material with the electric and magnetic dipole moments of the inclusions which can be calculated in a numerical or analytic way. Analysis of "meta-materials" is conducted to validate the proposed method.

Keywords: Bi-anisotropic material, Generalized Lorentz-Lorenz formula

1. INTRODUCTION

Developing artificial materials which have improved or new material properties that are not found in natural materials is a topic of continuing interest. Artificial dielectric materials have been explored for light-weight microwave antenna lenses, radar absorbing materials, substrates of electronic devices, and so on. The characterization of composite materials has been studied extensively for more than a century, and a number of effective medium theories have been proposed to calculate the effective permittivity of a composite which consists of a host medium and electrically small inclusions.[1–3] One of the deficiencies of effective medium models is their inability to integrate scattering characteristics of arbitrarily shaped particles such as rings and coils. Recently, a few numerical techniques have been proposed to deal with this problem.[4,5] However, most previous methods do not consider the combination of effective permittivity and permeability. In this paper, we present a combined numerical and analytic scheme to calculate constitutive relations for bi-anisotropic composite materials. We make use of the general formulation we obtained previously.[6]

In 1999, Pendry et al. proposed a new composite material consisting of a three-dimensional array of non-magnetic conducting particles, and showed it can have very large positive and negative effective permeability by making the inclusions resonant.[7] Since then, this new material, called "meta-material", has attracted many researchers' attention because the material with a negative permeability has never been found before and a "left-handed medium"[8] which has simultaneous negative permittivity and permeability, therefore, has a negative refractive index, can be constructed with the meta-material. Several experimental and numerical approaches have been made either to validate the characteristics of the meta-materials or to study the new and interesting phenomena introduced by "left-handed" properties.[9–12] To investigate this type of new composite materials efficiently, it is important to describe the material characteristics in terms of the physical properties of the inclusions which may have complicated geometries.

Further author information: (Send correspondence to S.-W. Lee)

S.-W. Lee: E-mail: lsw@ee.washington.edu, Telephone: 1 206 543 2159

A. Ishimaru: E-mail: ishimaru@ee.washington.edu, Telephone: 1 206 543 2169

Y. Kuga: E-mail: kuga@ee.washington.edu, Telephone: 1 206 543 0478

V. Jandhyala: E-mail: jandhyala@ee.washington.edu, Telephone: 1 206 543 2186

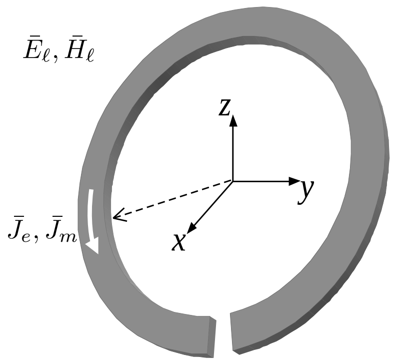


Figure 1. Currents $\bar{J}_e$ and $\bar{J}_m$ on the inclusion produced by the local fields $\bar{E}_\ell$ and $\bar{H}_\ell$ respectively.

This paper presents a generalized matrix representation of the macroscopic constitutive relations based on the quasi-static Lorentz-Lorenz theory. The constitutive relations are given by

$$\begin{bmatrix} \bar{D} \\ \bar{B} \end{bmatrix} = \begin{bmatrix} \bar{\bar{\epsilon}} & \bar{\bar{\xi}} \\ \bar{\bar{\zeta}} & \bar{\bar{\mu}} \end{bmatrix} \begin{bmatrix} \bar{E} \\ \bar{H} \end{bmatrix} \tag{1}$$

where $\bar{\bar{\epsilon}}$, $\bar{\bar{\xi}}$, $\bar{\bar{\zeta}}$, and $\bar{\bar{\mu}}$ are 3×3 matrices. In the next section, we derive the explicit expressions of all these matrix parameters for a given configuration of the inclusions in a host medium. The inclusions are arranged in a three-dimensional array and consist of non-magnetic materials with complex dielectric constants. The derivation is based on the quasi-static Lorentz-Lorenz theory and, therefore, applicable to inclusions whose sizes and spacings are small compared with a wavelength.

2. FORMULATION OF THE PROBLEM

This section describes the formulation which we obtained previously,[6] and it is repeated here for completeness. Under the quasi-static approximation, the electric and magnetic dipole moments, $\bar{p}_e$ and $\bar{p}_m$ of each inclusion are produced by the local fields $[\bar{E}_\ell \; \bar{H}_\ell]^{\mathrm{T}}$ which are the fields due to all other dipoles surrounding that particular inclusion. The dipole moments are then given by the generalized polarizability matrix $[\bar{\bar{\alpha}}]$.

$$\begin{bmatrix} \bar{p}_e \\ \bar{p}_m \end{bmatrix} = [\bar{\bar{\alpha}}] \begin{bmatrix} \bar{E}_\ell \\ \bar{H}_\ell \end{bmatrix} \tag{2}$$

where $[\bar{\bar{\alpha}}] = \begin{bmatrix} \bar{\bar{\alpha}}_{ee} & \bar{\bar{\alpha}}_{em} \\ \bar{\bar{\alpha}}_{me} & \bar{\bar{\alpha}}_{mm} \end{bmatrix}$.
Note that $\bar{p}_e$, $\bar{p}_m$, $\bar{E}_\ell$, and $\bar{H}_\ell$ are all 3×1 vectors and $[\bar{\bar{\alpha}}]$ is a 6×6 matrix.

Let us examine the polarizability matrix $[\bar{\bar{\alpha}}]$. Consider the x-component $E_{\ell x}$ of the local field $\bar{E}_\ell$. This field $E_{\ell x}$ is incident upon the inclusion and produces the current $\bar{J}_x E_{\ell x}$, which in turn produces the electric dipole moment $\bar{p}_e$ and the magnetic dipole moment $\bar{p}_m$ given by (Fig. 1).

$$\begin{aligned} \bar{p}_e &= \frac{1}{j\omega}\int \bar{J}_x \; dv \; E_{\ell x} \\ \bar{p}_m &= \frac{\mu_0}{2}\int \bar{r}\times\bar{J}_x \; dv \; E_{\ell x} \end{aligned} \tag{3}$$

$\bar{J}_x$ is the current produced by $E_{\ell x}$ and has three components J_{xx}, J_{yx}, and J_{zx}. And, therefore, we can write in the matrix form:

$$\begin{bmatrix} p_{ex} \\ p_{ey} \\ p_{ez} \end{bmatrix} = \frac{1}{j\omega}\int dv \begin{bmatrix} J_{xx} & J_{xy} & J_{xz} \\ J_{yx} & J_{yy} & J_{yz} \\ J_{zx} & J_{zy} & J_{zz} \end{bmatrix} \begin{bmatrix} E_{\ell x} \\ E_{\ell y} \\ E_{\ell z} \end{bmatrix}. \tag{4}$$

We express this as

$$[\bar{p}_e] = \frac{1}{j\omega}\int dv\ [\bar{J}_e][\bar{E}_\ell]. \tag{5}$$

The current $\bar{J}_e$ also produces the magnetic dipole moment.

$$[\bar{p}_m] = \frac{\mu_0}{2}\int dv\ \bar{r}\times[\bar{J}_e][\bar{E}_\ell]. \tag{6}$$

Next consider the magnetic local field $\bar{H}_\ell$, which produces the current $\bar{J}_m$. This also produces the electric and the magnetic dipole moments. Thus, we have

$$[\bar{p}_e] = \frac{1}{j\omega}\int dv\ [\bar{J}_m][\bar{H}_\ell], \tag{7}$$

$$[\bar{p}_m] = \frac{\mu_0}{2}\int dv\ \bar{r}\times[\bar{J}_m][\bar{H}_\ell]. \tag{8}$$

Now we have the final expressions for all the components of the polarizability matrix $[\bar{\bar{\alpha}}]$.

$$\begin{aligned}
\bar{\bar{\alpha}}_{ee} &= \frac{1}{j\omega}\int dv\ [\bar{J}_e] \\
\bar{\bar{\alpha}}_{me} &= \frac{\mu_0}{2}\int dv\ \bar{r}\times[\bar{J}_e] \\
\bar{\bar{\alpha}}_{em} &= \frac{1}{j\omega}\int dv\ [\bar{J}_m] \\
\bar{\bar{\alpha}}_{mm} &= \frac{\mu_0}{2}\int dv\ \bar{r}\times[\bar{J}_m].
\end{aligned} \tag{9}$$

Let us next consider the local fields $[\bar{E}_\ell\ \bar{H}_\ell]^{\mathrm{T}}$. As discussed above, the local fields act on the inclusion and produce the electric and magnetic dipoles. The local fields consist of the applied fields $[\bar{E}\ \bar{H}]^{\mathrm{T}}$ and the interaction fields $[\bar{E}_i\ \bar{H}_i]^{\mathrm{T}}$.

$$\begin{bmatrix}\bar{E}_\ell \\ \bar{H}_\ell\end{bmatrix} = \begin{bmatrix}\bar{E} \\ \bar{H}\end{bmatrix} + \begin{bmatrix}\bar{E}_i \\ \bar{H}_i\end{bmatrix}. \tag{10}$$

The interaction fields are produced by all the dipoles except those of the particular inclusion under consideration. For a three-dimensional array of inclusions, the interaction fields $[\bar{E}_i\ \bar{H}_i]^{\mathrm{T}}$ have been obtained and are given by

$$\begin{bmatrix}\bar{E}_i \\ \bar{H}_i\end{bmatrix} = \mathrm{N}\begin{bmatrix}\frac{1}{\epsilon_0}\bar{\mathrm{C}} & \bar{0} \\ \bar{0} & \frac{1}{\mu_0}\bar{\mathrm{C}}\end{bmatrix}\begin{bmatrix}\bar{p}_e \\ \bar{p}_m\end{bmatrix} \tag{11}$$

where N is the number of inclusions per unit volume and is equal to $\mathrm{N} = (abc)^{-1}$, and $[\bar{\mathrm{C}}]$ is the interaction constant matrix which is given by

$$\bar{\mathrm{C}} = \begin{bmatrix}\mathrm{C}_x & 0 & 0 \\ 0 & \mathrm{C}_y & 0 \\ 0 & 0 & \mathrm{C}_z\end{bmatrix}, \tag{12}$$

and $\bar{0}$ is a 3×3 null matrix. The interaction constant matrix $[\bar{\mathrm{C}}]$ for a three-dimensional array of dipoles with the spacings a, b, and c in the x, y, and z directions respectively (Fig. 2), has been obtained.[13]

$$\begin{aligned}
\mathrm{C}_x &= f\left(\frac{b}{a}, \frac{c}{a}\right) = \left(\frac{b}{a}\right)\left(\frac{c}{a}\right)\left[\frac{1.202}{\pi} - S\left(\frac{b}{a}, \frac{c}{a}\right)\right] \\
\mathrm{C}_y &= f\left(\frac{c}{b}, \frac{a}{b}\right) \\
\mathrm{C}_z &= f\left(\frac{a}{c}, \frac{b}{c}\right)
\end{aligned} \tag{13}$$

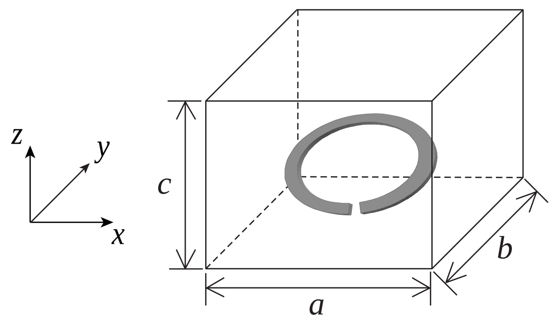


Figure 2. Unit cell in a three-dimensional array of inclusions with the spacing a, b, and c in the x, y, and z directions respectively.

where

$$S\left(\frac{b}{a},\frac{c}{a}\right) = \frac{1}{\pi}\sum_{n=-\infty}^{\infty}\sum_{s=-\infty}^{\infty}\sum_{m=1}^{\infty}(2m\pi)^2\ \mathrm{K}_0\left(2m\pi\left[\left(\frac{nb}{a}\right)^2+\left(\frac{sc}{a}\right)^2\right]^{1/2}\right),$$

K_0 is the modified Bessel function, and the term with $n = s = 0$ is excluded.

Substituting (2) and (11) into (10), we obtain

$$\begin{bmatrix}\bar{E}_\ell\\ \bar{H}_\ell\end{bmatrix} = \begin{bmatrix}\bar{E}\\ \bar{H}\end{bmatrix} + \mathrm{N}\begin{bmatrix}\frac{1}{\epsilon_0}\bar{\mathrm{C}} & \bar{0}\\ \bar{0} & \frac{1}{\mu_0}\bar{\mathrm{C}}\end{bmatrix}[\bar{\bar{\alpha}}]\begin{bmatrix}\bar{E}_\ell\\ \bar{H}_\ell\end{bmatrix}. \tag{14}$$

We then obtain

$$\begin{bmatrix}\bar{E}_\ell\\ \bar{H}_\ell\end{bmatrix} = \left[\begin{bmatrix}\bar{\mathrm{U}} & \bar{0}\\ \bar{0} & \bar{\mathrm{U}}\end{bmatrix} - \mathrm{N}\begin{bmatrix}\frac{1}{\epsilon_0}\bar{\mathrm{C}} & \bar{0}\\ \bar{0} & \frac{1}{\mu_0}\bar{\mathrm{C}}\end{bmatrix}[\bar{\bar{\alpha}}]\right]^{-1}\begin{bmatrix}\bar{E}\\ \bar{H}\end{bmatrix} \tag{15}$$

where $[\bar{\mathrm{U}}]$ is a 3×3 unit matrix. Finally, $\bar{D}$ and $\bar{B}$ are given by

$$\begin{bmatrix}\bar{D}\\ \bar{B}\end{bmatrix} = \begin{bmatrix}\epsilon_0\bar{E}\\ \mu_0\bar{H}\end{bmatrix} + \mathrm{N}\begin{bmatrix}\bar{p}_e\\ \bar{p}_m\end{bmatrix}. \tag{16}$$

Substituting (2) and (15) into (16), we get

$$\begin{bmatrix}\bar{D}\\ \bar{B}\end{bmatrix} = \begin{bmatrix}\bar{\bar{\epsilon}} & \bar{\bar{\xi}}\\ \bar{\bar{\zeta}} & \bar{\bar{\mu}}\end{bmatrix}\begin{bmatrix}\bar{E}\\ \bar{H}\end{bmatrix}$$

where

$$\begin{bmatrix}\bar{\bar{\epsilon}} & \bar{\bar{\xi}}\\ \bar{\bar{\zeta}} & \bar{\bar{\mu}}\end{bmatrix} = \begin{bmatrix}\epsilon_0\bar{\mathrm{U}} & \bar{0}\\ \bar{0} & \mu_0\bar{\mathrm{U}}\end{bmatrix} + \mathrm{N}\,[\bar{\bar{\alpha}}]\left[\begin{bmatrix}\bar{\mathrm{U}} & \bar{0}\\ \bar{0} & \bar{\mathrm{U}}\end{bmatrix} - \mathrm{N}\begin{bmatrix}\frac{1}{\epsilon_0}\bar{\mathrm{C}} & \bar{0}\\ \bar{0} & \frac{1}{\mu_0}\bar{\mathrm{C}}\end{bmatrix}[\bar{\bar{\alpha}}]\right]^{-1}. \tag{17}$$

This is the final expression for the generalized constitutive relations for a three-dimensional array of inclusions under the quasi-static approximation. This is the generalization of the Lorentz-Lorenz formula and leads to the Maxwell-Garnett formula for spherical inclusions.

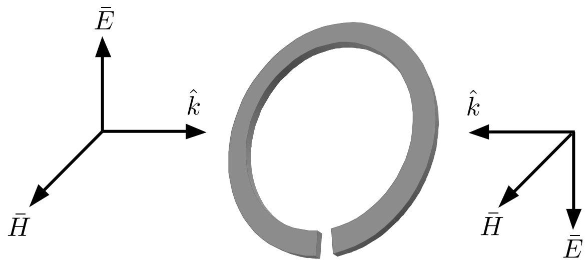


Figure 3. Incident plane waves from two symmetric directions produce an almost uniform magnetic field on the inclusion.

3. QUASI-STATIC CALCULATION OF $\bar{\mathbf{J}}_{\mathbf{E}}$ AND $\bar{\mathbf{J}}_{\mathbf{M}}$

As can be seen from (5), (6), (7), and (8), the current $\bar{J}_e$ on the inclusion is produced by $\bar{E}_\ell$, and the current $\bar{J}_m$ is produced by $\bar{H}_\ell$, and these two currents are independently produced under the quasi-static approximation.

In order to calculate $\bar{J}_m$, we apply a uniform magnetic field on the inclusion and calculate the current. For example, for the magnetic field $\bar{H}_\ell = H_0\hat{z}$, we need to have the incident field H_0 which is uniform throughout the space $a \times b \times c$. Since electromagnetic codes are available which can calculate the current on the inclusion with a plane wave incidence, it is convenient to make use of these existing codes. Ansoft HFSS 8.0 is used for our work. However, a plane wave does not give a uniform magnetic field. To obtain a uniform magnetic field, we use the incident plane waves from several symmetric directions as shown in Fig. 3. The electric field at or near the inclusion is canceled out and nearly zero, and the magnetic field is close to uniform. The current $\bar{J}_m$ is then numerically calculated. To produce a uniform $\bar{E}_\ell$, anti-symmetric plane wave excitation is used.

It should be pointed out that the magnetic polarizability (9) is given by the volume integral of the form:

$$\int dv\ \bar{r} \times \bar{J}. \tag{18}$$

Even though this is independent of the choice of origin for the magnetostatic case where $\nabla \cdot \bar{J} = 0$, in general, this integral depends on the choice of origin. Therefore, the origin should be chosen at the center of gravity of the geometric shape of the inclusion.

4. COMPUTATION RESULTS

To illustrate the usefulness of the proposed method, we consider Pendry et al.'s split ring resonator (SRR) structures (Fig. 4).[7] Using the scheme shown in Fig. 3, we calculate μ' and μ'', which are shown in Fig. 5(a). The effective permeability of the SRR structure has been studied by Pendry et al., and the following expression was derived.

$$\mu_{\text{eff}} = \mu' - j\mu'' = 1 - \frac{\dfrac{\pi r^2}{a^2}}{1 - \dfrac{2l\rho}{\omega r \mu_0} j - \dfrac{3lc_0^2}{\pi\omega^2 \ln\dfrac{2w}{d} r^3}} \tag{19}$$

where ρ is the resistance per unit length of the rings measured around the circumference and c_0 is the velocity of light, and the underlying assumptions of the above equation are

$$\begin{aligned} r &\gg w, \qquad r \gg d, \\ l &< r, \\ \ln\frac{w}{d} &\gg \pi. \end{aligned} \tag{20}$$

In Fig. 5(b), μ' and μ'' obtained using the above equation are shown. Two calculated results showed very similar behavior, although there is a difference between the resonant frequencies. It should be noted that the

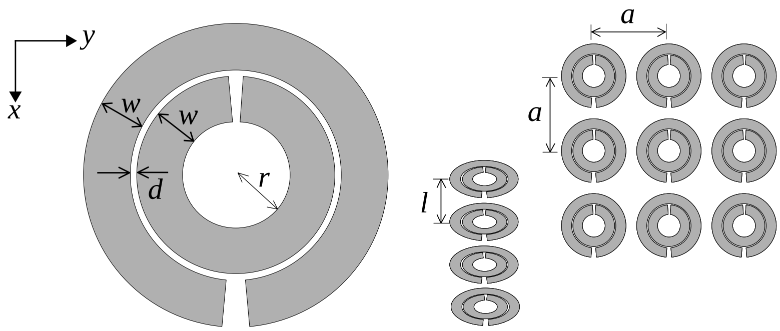
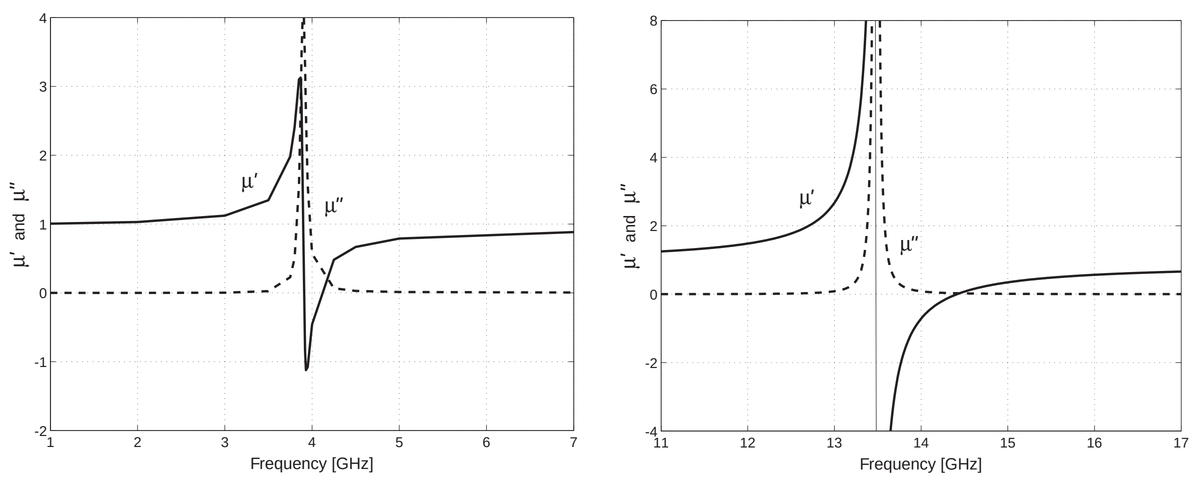


Figure 4. Split ring resonator (SRR) and definitions of distances.

SRR parameters used for current calculation do not satisfy the above inequalities which are important for the accuracy of the formula, and it may cause the discrepancy.

We conduct another computation with different SRR dimensions which were used in Ref. 9, where the resonant frequency has been obtained in both numerical and experimental ways, and it is 4.845GHz. Fig. 6(a) shows this value agrees with our calculation. We also calculate ϵ' and ϵ'' ($\epsilon_{\text{eff}} = \epsilon' - j\epsilon''$), which are shown in Fig. 6(b). For this simulation, only $E_{\ell x}$, $E_{\ell y}$, and $H_{\ell z}$ are considered and, therefore, ϵ_{xx}, ϵ_{yy}, and μ_{zz} are calculated. Note that ϵ_{yy} also shows an analogous resonance curve to that of μ_{zz} whereas ϵ_{xx} is almost constant. This fact implies that the SRR structure itself can form the left-handed medium, while it has been believed that this can be done only when combined with another unit with a negative permittivity.

For the last simulation, we analyze a stacked SRR structure in which one split ring is placed at the top of the other split ring (Fig. 7). ϵ_{xx}, ϵ_{yy}, and μ_{zz} of this stacked SRR structure are calculated and plotted in Fig. 8. It is clear that ϵ_{yy} does not have a resonance unlike that of the ordinary SRR strucure, while ϵ_{xx} and μ_{zz} show similar characteristics. Further research may utilize this difference to verify the left-handed properties of the SRR structures.



(a) (b)

Figure 5. Plot of μ of Pendry et al.'s SRR structure. $r = 2$mm, $w = 1$mm, $d = 0.1$mm, $a = 10$mm, and $l = 3$mm. The conductivity of the ring is 5.8×10^7[S/m]. (a) Proposed method (b) Pendry et al.'s formula

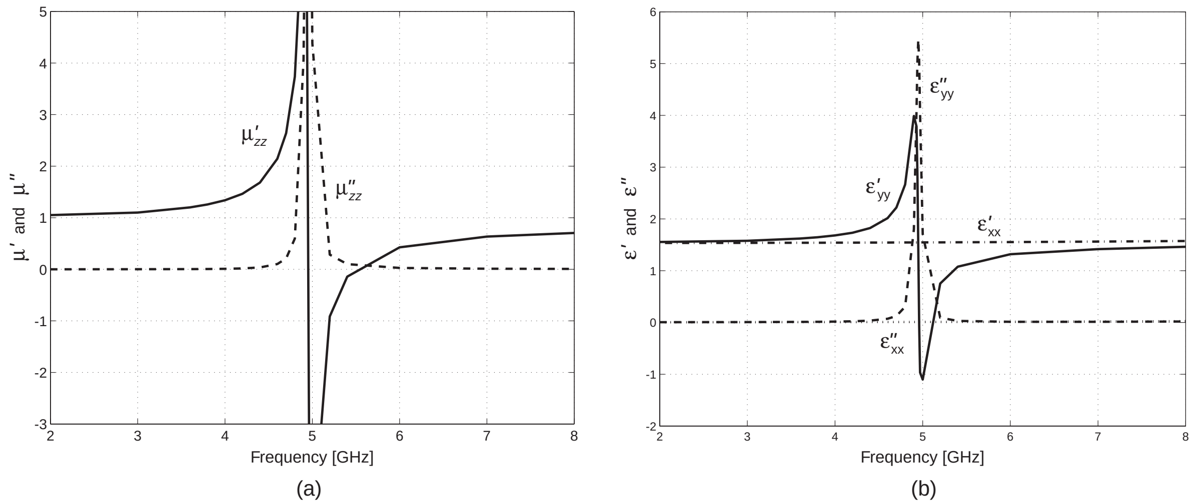


Figure 6. Plot of μ and ϵ of Smith et al.'s SRR structure. r = 1.5mm, w = 0.8mm, d = 0.2mm, a = 8mm, and l = 3.2mm. The conductivity of the ring is 5.8×10^7[S/m].

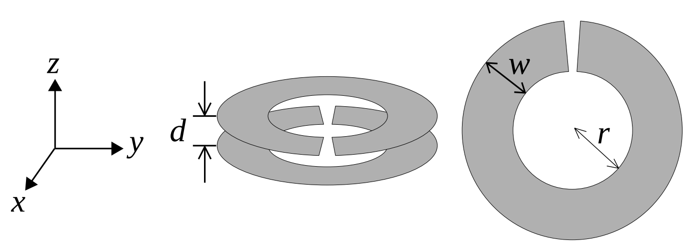


Figure 7. Stacked split ring resonator and definitions of dimensions.

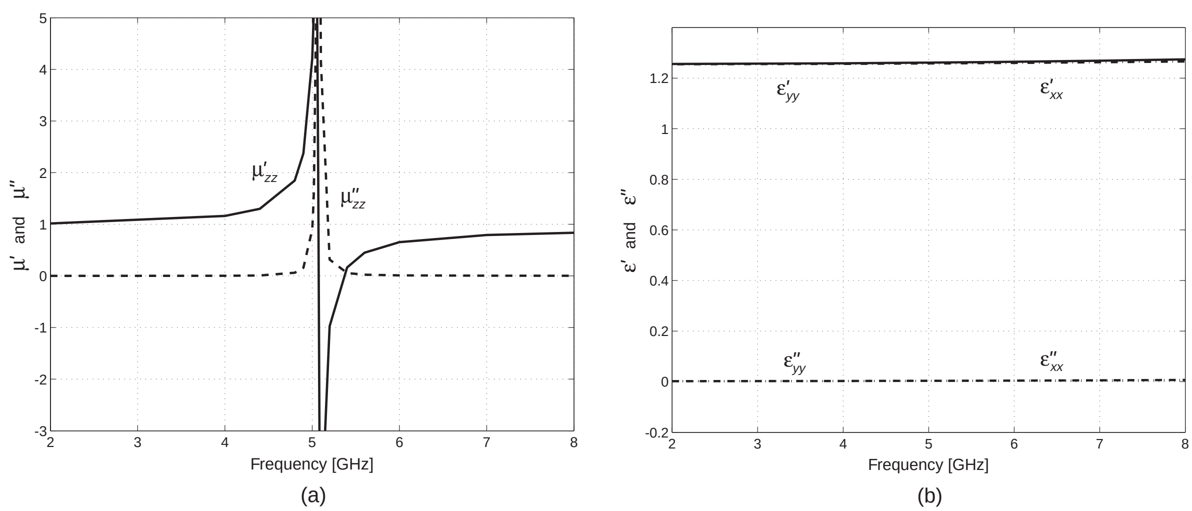


Figure 8. Plot of μ and ϵ of the stacked split ring resonator structure. r = 1.5mm, w = 0.8mm, d = 0.2mm, a = 8mm, and l = 3.2mm. The conductivity of the ring is 5.8×10^7[S/m].

5. CONCLUSIONS

In this paper, we presented a combined numerical and analytic approach to obtain the generalized constitutive relations (17) for bi-anisotropic materials consisting of a three-dimensional array of inclusions of arbitrary shapes. This method is based on the quasi-static approximation and, therefore, is applicable to inclusions whose sizes and spacings are small compared with a wavelength. Several numerical examples including split ring resonator structures are shown to illustrate the usefulness of the formulation.

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REFERENCES

1. W. T. Doyle, "Particle clustering and dielectric enhancement in percolating metal-insulator composites," *J. Appl. Phys.*, **78**, pp. 6165–6169, 1995.
2. W. T. Doyle, "Electrical and optical properties of dense composites," *J. Appl. Phys.*, **85**, pp. 2323–2329, 1999.
3. A. J. Stoyanov, B. F. Howell, E. C. Fischer, H. Überall, and K. Chouffani, "Effective-medium model dependence of the radar reflectivity of conducting particle films," *J. Appl. Phys.*, **86**, pp. 3110–3119, 1999.
4. F. Wu and K. W. Whites, "Quasi-static effective permittivity of periodic composites containing complex shaped dielectric particles," *IEEE Trans. Antennas Propag.*, **49**, pp. 1174–1182, August 2001.
5. B. Sareni, L. Krähenbühl, A. Beroual, and A. Nicolas, "A boundary integral equation method for the calculation of the effective permittivity of periodic composites," *IEEE Trans. Magn.*, **33**, pp. 1580–1583, 1997.
6. A. Ishimaru, S.-W. Lee, Y. Kuga, and V. Jandhyala, "Generalized constitutive relations for meta-materials based on the quasi-static Lorentz-Lorenz theory," submitted to *IEEE Trans. Antennas Propag.*, 2002.
7. J. B. Pendry, A. J. Holden, D. J. Robbins, and W. J. Stewart, "Magnetism from conductors and enhanced nonlinear phenomena," *IEEE Trans. Microwave Theory Tech.*, **47**, pp. 2075–2084, 1999.
8. V. G. Vesalago, "The electrodynamics of substances with simultaneously negative values of ϵ and μ," *Sov. Phys. Usp.*, **10**, pp. 509–514, 1968.
9. D. R. Smith, W. J. Padilla, D. C. Vier, S. C. Nemat-Nasser, and S. Schultz, "Composite medium with simultaneously negative permeability and permittivity," *Phys. Rev. Lett.*, **84**, pp. 4184–4187, 2000.
10. J. B. Pendry, "Negative refraction makes a perfect lens," *Phys. Rev. Lett.*, **85**, pp. 3966–3969, 2000.
11. R. W. Ziolkowski and E. Heyman, "Wave propagation in media having negative permittivity and permeability," *Phys. Rev. E*, **64**, 056625, 2001.
12. R. A. Shelby, D. R. Smith, and S. Schultz, "Experimental verification of a negative index of refraction," *Science*, **292**, pp. 77–79, 2001.
13. R. E. Collin, *Field Theory of Guided Waves*, Chapter 12, IEEE Press, N.Y. 1991.