Homogenization of 3-D Periodic Bianisotropic Metamaterials

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***Abstract*—A novel homogenization technique, combining an asymptotic multiscale method with wave-field conception, is proposed for computing the quasi-static effective parameters of three-dimensional lattices of general bianisotropic composite materials. This technique is based on the decomposition of the fields into an averaged nonoscillating part and a corrected term with microoscillation. This paper provides an original and accurate way to model the electromagnetic fields in fine microstructures of bianisotropic particles with complex inclusion shapes when the wavelength is larger than the periodicity of the microstructure. The effects of the interaction between edges and corners of adjacent inclusions on the macroscopic effective parameters have been studied, and numerical results and verifications have been presented.**

***Index Terms*—Bianisotropic composites, chiral composites, effective parameters, finite-element method (FEM), homogenization, metamaterials, microstructure.**

I. Introduction

COMPOSITE structured materials have attracted growing interest in recent years due to their potential applications such as optical waveguides, high-dielectric thin-film capacitors, captive video disk units, and novel antennas [1]–[3]. Recently, a new class of these structured materials *metamaterials* with simultaneously negative permittivity and permeability has inspired great interests in their unique physical properties [3]–[6]. They have shown great potential in many applications such as super lenses, filters, subwavelength resonant cavities, waveguides, and antennas. It is of particular interest to consider the bianisotropy [7], [8] of the metamaterials, such as the design of complementary split-ring resonators (SRRs) [9] and extraction of bianisotropic constitutive parameters for SRR-based metamaterials from S-parameters [10]. It was recently shown that negative refraction can be achieved by materials with positive parameters provided one of the materials is chiral or gyrotropic [11], [12].

A central problem in the theory of composites is the study of how physical properties of composites such as permittivity and permeability depend on the properties of their constituents. In general, these properties strongly depend on the microstructure. To predict the effective electromagnetic (EM) properties of structured artificial materials, especially when the wavelength is larger than the periodicity, there are analytical formulation such as Maxwell Garnett and Bruggeman mixing formulas [13] and some numerical techniques such as the boundary integral-equation method, method of moments, and finite-element method (FEM) [14], [15]. Note that most of the methods aforementioned, which describe the dielectric responses of each particle and mutual interaction among inclusions, are developed and applicable only for very simple shapes with very weak interaction or simple isotropic or anisotropic material constitutions. This motivates this paper, which proposes a method to compute the effective constitutive parameters for the most general bianisotropic composites with complex shaped inclusions. More importantly, this novel method can also precisely approximate the fields in finite lattices of periodic bianisotropic materials. The fields are computed only in the unit cell and then generalized over the whole volume. Therefore, given a large finite lattice of bianisotropic composites, the time of computation and the memory requirement can be greatly reduced without the loss of accuracy. The proposed methodology for homogenization, which is a development of our previous study devoted to lossy anisotropic periodic microstructures [17], is not based on an averaging operation (e.g., Maxwell-Garnett (M–G) and Bruggeman mixing rules), but stems from a rigorous limit process. The proposed advanced homogenization method can be applied not only to general bianisotropic composite media, but also to arbitrarily shaped inclusions. Hence, this paper goes a step further in the development of the homogenization method for composite metamaterials.

This paper is organized as follows. In Section II, a short summary of the asymptotic multiscale theory of homogenization applied to general bianisotropic is given. In Section III, various chiral inclusions with complex shapes (with convex and concave contours) have been numerically studied to understand the influence of corners and edges of the inclusions on the effective parameters. The effective parameters of bianisotropic inclusions embedded in bianisotropic host media are also presented. EM wave propagation in a finite lattice of cubic chiral objects is studied, and good agreement is observed by comparing the current method and direct FEM. Finally, conclusions are drawn in Section IV.

II. Formulation

We consider a periodic structure of identical bianisotropic inclusions immersed in a homogeneous host medium. The constitutive relations of the bianisotropic media are given, in the time dependence of $e^{i\omega t}$, as follows:

$$\begin{cases} \vec{D} = \overline{\overline{\varepsilon}} \cdot \vec{E} + \sqrt{\varepsilon_0\mu_0}\,\overline{\overline{\xi}} \cdot \vec{H} \\ \vec{B} = \sqrt{\varepsilon_0\mu_0}\,\overline{\overline{\varsigma}} \cdot \vec{E} + \overline{\overline{\mu}} \cdot \vec{H} \end{cases} \tag{1}$$

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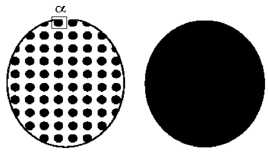

Fig. 1. (a) Periodic composite material. (b) Same material when the periodicity α tends to zero.

where the four material parameter dyadics are permittivity $\overline{\overline{\varepsilon}}$ and permeability $\overline{\overline{\mu}}$, and two cross-polarization dyadics $\overline{\overline{\xi}}$ and $\overline{\overline{\varsigma}}$. The reference unit cell is characterized by Y^α with the cell's periodicity α and scaled unit cell αY, where Y is the unit volume of the cubes in three-dimensional (3-D) spaces. The configuration is shown in Fig. 1(a).

It is well known that, for isotropic dielectric materials, source-incorporated Maxwell equations can be expressed as follows:

$$\begin{cases} \nabla \times \vec{E}^\alpha(x) = -\dfrac{\partial \vec{B}^\alpha(x)}{\partial t} \\ \nabla \times \vec{H}^\alpha(x) = \dfrac{\partial \vec{D}^\alpha(x)}{\partial t} + \vec{J}^\alpha(x) \end{cases} \tag{2}$$

where $\vec{E}^\alpha$ and $\vec{H}^\alpha$ represent the electric and magnetic fields, and $\vec{D}^\alpha$, $\vec{B}^\alpha$, and $\vec{J}^\alpha$ are, respectively, the electric displacement, magnetic induction, and excitation source. The variable x denotes the smooth variation of the field from cell to cell. Spatial functions of $\overline{\overline{\varepsilon}}$, $\overline{\overline{\mu}}$, $\overline{\overline{\xi}}$, and $\overline{\overline{\varsigma}}$ oscillate drastically in the considered structure due to the heterogeneities. These oscillations are difficult to treat numerically. Therefore, homogenization theory can be used to give the macroscopic global properties of the current composite by taking into account the properties of the microscopic structure. Hence, another variable $y = x/\alpha$ is introduced to describe the fast variation within the cell.

We can further rewrite (2) in matrix form

$$i\omega A^\alpha(y)u^\alpha(\omega, x) = Mu^\alpha(\omega, x) - J^\alpha(\omega, x) \tag{3}$$

where A^α is a $6 \cdot 6$ matrix comprised of the material parameters of the unit cell and M represents the rotational operator. When the period of the lattice is quite small compared to the wavelength, the total EM fields can thus be expanded by a function of an average part u with a series of corrector terms

$$u^\alpha(\omega, x) = u(\omega, x) + \nabla_y \Phi(\omega, x, y) + \alpha \Psi(\omega, x, y) + \cdots \tag{4}$$

where only the first two terms (i.e., macroscopic EM field $u(\omega, x)$ of the cell and the first microscopic corrector $\nabla_y \Phi(\omega, x, y)$) are required for computation. Strong convergence can be obtained without subsequent high-order corrector potentials [18], [19]. Thus, we obtain by taking the limit of α tending to zero in (3) [see Fig. 1(b)]

$$\begin{aligned} i\omega A(y)(u(\omega, x) + \nabla_y \Phi(\omega, x, y)) \\ = M_x u(\omega, x) + M_y \Phi(\omega, x, y) - J(\omega, x). \end{aligned} \tag{5}$$

Scalar-dotting a testing periodic function ϕ in its gradient form, we can arrive at the following equation after the integration over the whole volume is performed:

$$\begin{aligned} \int_Y i\omega A(y)(u(\omega, x) + \nabla_y \Phi(\omega, x, y)) \cdot \nabla_y \phi(y) dy \\ = \int_Y (M_x u(\omega, x) + M_y \Phi(\omega, x, y) - J(\omega, x)) \cdot \nabla_y \phi(y) dy. \end{aligned} \tag{6}$$

Due to the convergence theorem of the periodic function, it can be obtained for the right-hand-side term of (6) as follows:

$$\begin{aligned} \int_Y (M_x u(\omega, x) + M_y \Phi(\omega, x, y) - J(\omega, x)) \cdot \nabla_y \phi(y) dy \\ = -\int_Y \phi(y) \nabla_y (M_x u(\omega, x) + M_y \Phi(\omega, x, y) - J(\omega, x)) dy. \end{aligned} \tag{7}$$

Note that $M_x u(\omega, x) - J(\omega, x)$ is independent on the microscopic variable y and $\nabla_y \cdot M_y = 0$ (since M is a rotational operator). Therefore, the right-hand side of (7) is zero, and the integral of the limit (6) becomes

$$\int_Y [i\omega A(y)(u(\omega, x) + \nabla_y \Phi(\omega, x, y)) \cdot \nabla_y \phi(y)] dY = 0. \tag{8}$$

The term of $\Phi(\omega, x, y)$ and $\nabla_y \Phi(\omega, x, y)$ are then represented as

$$\Phi(\omega, x, y) = u(\omega, x)\psi(\omega, y) = \sum_{j=1}^{6} u_j(\omega, x)\psi_j(\omega, y) \tag{9a}$$

$$\nabla_y \Phi(\omega, x, y) = \sum_{j=1}^{6} u_j(\omega, x) \nabla_y \psi_j(\omega, y) \tag{9b}$$

thus $u + \nabla_y \Phi$ is given by

$$u + \nabla_y \Phi(\omega, x, y) = \sum_{j=1}^{6} u_j(\omega, x)(e_j + \nabla_y \psi_j(\omega, y)). \tag{9c}$$

When we insert (9c) in (8), we obtain that ψ_j ($j = 1, \ldots, 6$) is solution of the following equation:

$$\int_Y [A(y)(e_j + \nabla_y \psi_j(\omega, y)) \cdot \nabla_y \phi(y)] dY = 0. \tag{10}$$

Replacing $u + \nabla_y \Phi$ in the limit (3) by (9a) and integrating over the unit cell, we have

$$\begin{aligned} i\omega \int_Y A(y)[u(\omega, x) + u(\omega, x)\nabla_y \psi(\omega, y)] \cdot dy \\ = |Y| \, (Mu(\omega, x) - J(\omega, x)) \end{aligned} \tag{11}$$

where $|Y|$ is the volume of the unit cell ($|Y| = 1$). Thus, (11) can be expressed as

$$i\omega A_{\text{eff}} u(\omega, x) = Mu(\omega, x) - J(\omega, x) \tag{12}$$

where the macroscopic effective parameters in the dyadic form can be expressed as

$$A_{j,\text{eff}} = \int_Y [A(y)(e_j + \nabla_y \psi_j(\omega, y))] dy \tag{13}$$

where $A_{j,\mathrm{eff}}$ denotes the jth column of the $6 \cdot 6$ effective constitutive matrix $A(y)$, which is comprised of effective permittivity, permeability, and two cross-polarization dyadics.

The main advantage of this approach is that it gives the possibility to accurately evaluate the EM field inside finite lattices when the period of the lattice is small compared with that of the wavelength. This field is the sum of the average field and corrector field (9c). To validate this approach, the electric field in a finite periodic composite material with chiral properties is compared to that obtained by the method proposed in [20] combined with the FEM. In that method, a decomposition scheme is used to transform the chiral medium to their isotropic equivalences characterized by four equivalent permittivity/permeability parameters of $\varepsilon_\pm$ and $\mu_\pm$ as follows:

$$\begin{cases} \vec{D}_\pm = \varepsilon \vec{E}_\pm - i\kappa\sqrt{\varepsilon_0\mu_0}\vec{H}_\pm = \varepsilon_\pm \vec{E}_\pm \\ \vec{B}_\pm = i\kappa\sqrt{\varepsilon_0\mu_0}\vec{E}_\pm + \mu\vec{H}_\pm = \mu_\pm \vec{H}_\pm \end{cases} \tag{14}$$

where + and − denote right- and left-hand-side circular polarized eigenwaves inside the chiral medium, respectively. It can be verified that the respective equivalent permittivity $\varepsilon_\pm$ and permeability $\mu_\pm$ of the eigenmodes should agree with the following relation:

$$(\varepsilon - \varepsilon_\pm)(\mu - \mu_\pm) = \kappa^2 \varepsilon_0 \mu_0. \tag{15}$$

The wave fields $\vec{E}_\pm$ and $\vec{H}_\pm$ satisfy the Maxwell equations for isotropic dielectrics, as shown in (2), and we can obtain

$$\begin{cases} \varepsilon_\pm = \varepsilon\left(1 \pm \dfrac{\kappa\sqrt{\varepsilon_0\mu_0}}{\sqrt{\varepsilon\mu}}\right) \\ \mu_\pm = \mu\left(1 \pm \dfrac{\kappa\sqrt{\varepsilon_0\mu_0}}{\sqrt{\varepsilon\mu}}\right). \end{cases} \tag{16}$$

Now the chiral media can be regarded as a summation of effects from two fictional isotropic achiral materials characterized by (ε_+, μ_+) and (ε_-, μ_-), while the same excitation should be imposed for each of these two fictional cases. This method is significantly important to calculate the electric field because it can remove the term of $\nabla \times \vec{E}$ from the Helmholtz equations for chiral media, which greatly simplified the numerical computation.

III. Numerical Validation and Results

A. Effective Constitutive Parameters

Let us first consider infinite lattices of identical chiral cylinder inclusions of various cross sections (see Fig. 2) with relative permittivity and permeability $\varepsilon_r = \mu_r = 10$ and relative chirality $\kappa = 1$. The host medium is free space. The effects of the edges and discontinuities of the considered chiral inclusions are studied, which, originally, cannot be taken into account in the classical theory of homogenization (e.g., M–G formulas). Homogenized effective parameters are plotted against the volume fraction. We find that, for a lattice of square chiral cylinders, our current method surprisingly produces almost the same effective parameters as M–G formulas, which is best suited for smooth canonical shapes (i.e., ellipsoids). It was shown that, for this shape, the interaction of corners between adjacent inclusions becomes strong and enhances the depolarization of the

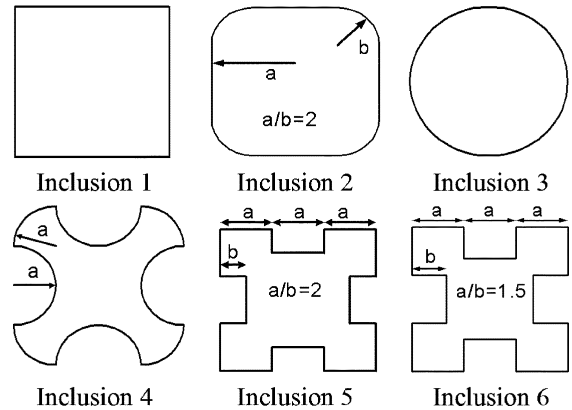

Fig. 2. Geometry of the studied two-dimensional inclusions.

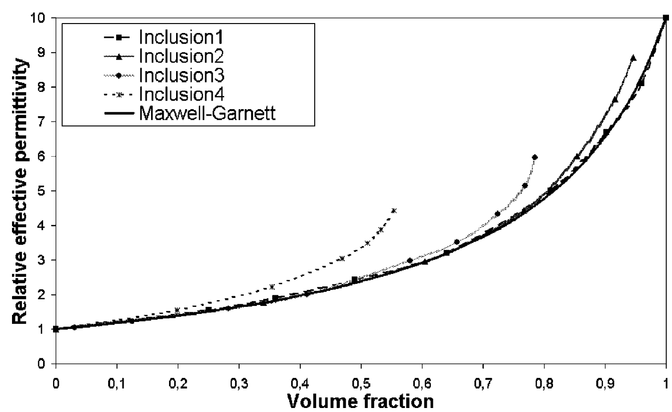

Fig. 3. Computed effective relative permittivity $\varepsilon_{r\mathrm{eff}}$ for square lattices of inclusions 1–4 ($\varepsilon_r = 10$) suspended in free space.

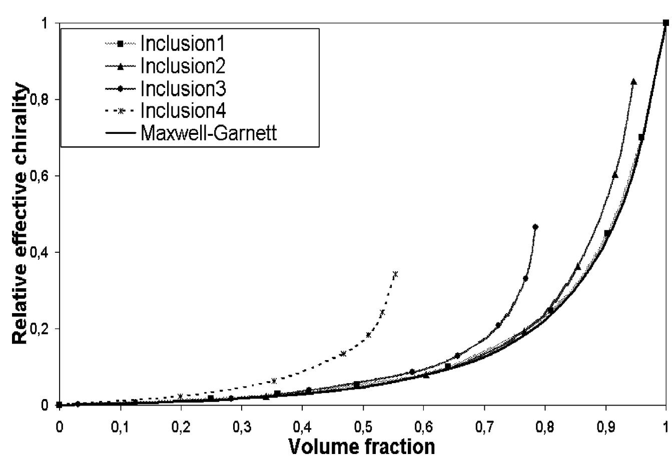

Fig. 4. Effective relative chirality κ_{eff} for square lattices of inclusions 1–4 ($\kappa = 1$) suspended in free space.

material, which results in the decrease of the effective parameters compared to other shapes [16].

In Figs. 3 and 4, we present the comparison of inclusions with different rounded corners and contours. One can see that, at the same fraction index, the inclusion with rounded concave contours (inclusion 4) gives the biggest effective permittivity and chirality. For a volume fraction bigger than 0.15, the difference between the curve of inclusion 4 and the other three curves of inclusions 1–3 becomes visibly larger and larger, which means the depolarization produced by the corners of inclusion 4 is much

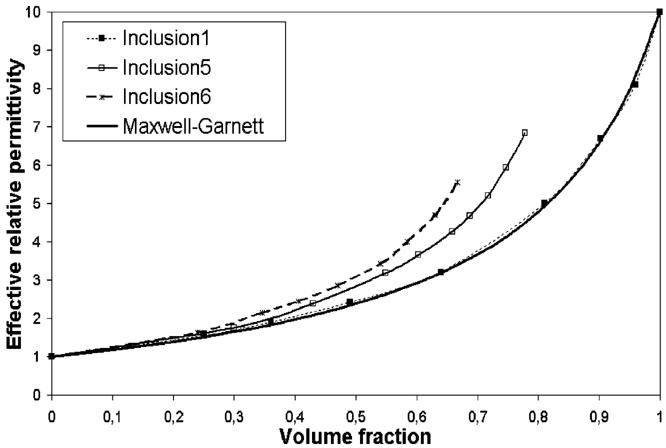

Fig. 5. Effective relative permittivity $\varepsilon_{r\text{eff}}$ for square lattices of inclusions 1, 5, and 6 ($\varepsilon_r = 10$) suspended in free space.

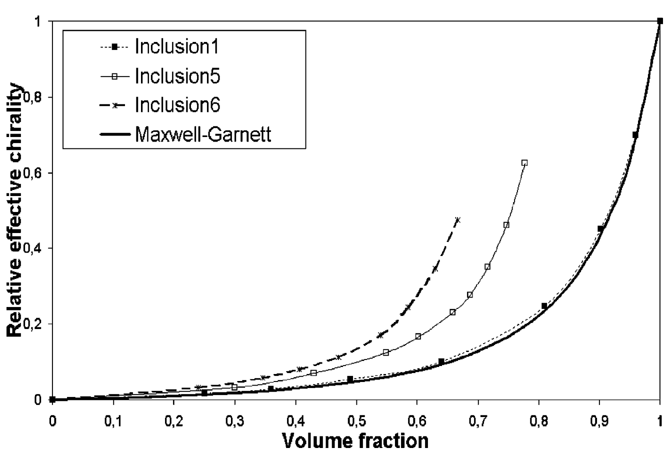

Fig. 6. Computed effective relative chirality κ_{eff} for square lattices of inclusions 1, 5, and 6 ($\kappa = 1$) suspended in free space.

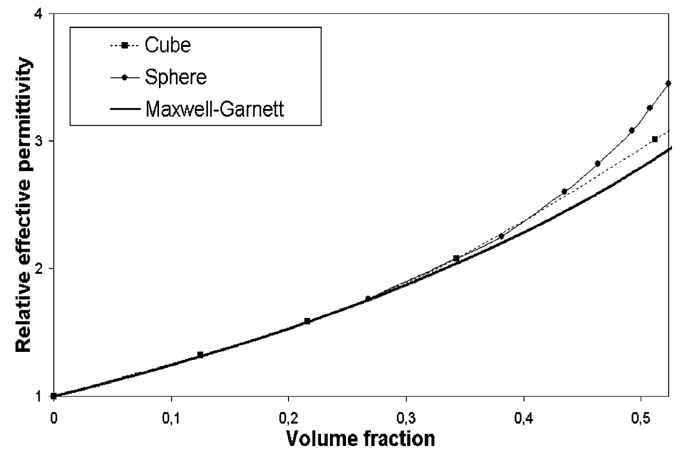

Fig. 7. Effective relative permittivity $\varepsilon_{r\text{eff}}$ for square lattices of spherical and cubical inclusions ($\varepsilon_r = 10$) suspended in free space.

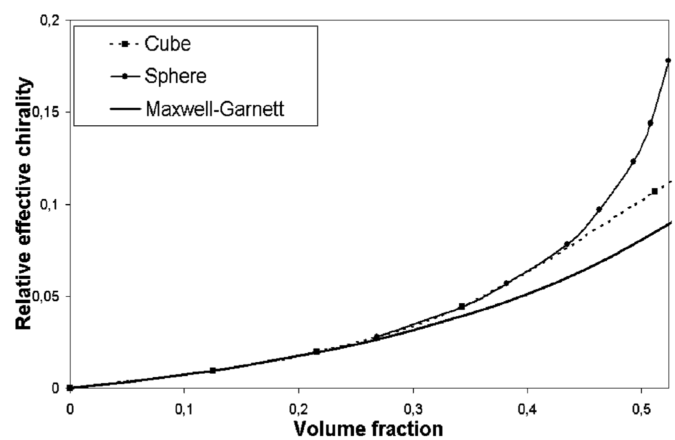

Fig. 8. Effective relative chirality κ_{eff} for square lattices of spherical and cubical inclusions ($\kappa = 1$) suspended in free space.

more decreased and high mutual coupling causes a bigger increase in the polarizability density than the other three inclusions. For each inclusion type, the effective parameters reach the upper limits with the maximum available volume fraction. A tradeoff can be observed between the effective parameters and volume fraction. For instance, when it is required to achieve a higher effective parameter, we need to embed more chiral inclusions per unit volume, or use complex shaped inclusions. If the parameter requirement is not very high, inclusion 4 will be a good choice to save materials.

In Figs. 5 and 6, we study the responses of chiral inclusions with different concavities. At a fixed fraction, the effective parameters of the inclusion with the biggest concavity are the largest. By comparison with Figs. 3 and 4, one can observe that the limit values for concave square chiral inclusions with corners are higher than the rounded concave ones. For example, at $f = 0.778$, we have $\varepsilon_{\text{eff}} = 5.717$ (Fig. 3) and $\kappa_{\text{eff}} = 0.416$ (Fig. 4) for inclusion 3, but $\varepsilon_{\text{eff}} = 6.84$ (Fig. 5) and $\kappa_{\text{eff}} = 0.625$ (Fig. 6) for inclusion 5. From Figs. 5 and 6, it can also be found that effective parameters will increase with the etching ratio b/a (for inclusions 1, 5, and 6, the etching ratio is 0, 0.5, and 0.667, respectively).

We utilize our method to compute for the 3-D spherical/cubic chiral inclusions, and compare with the results from the M-G formulas. We plot Figs. 7 and 8 over the volume fraction from 0 to 0.52, where $f_{\max}$ is reached for the lattice of chiral spheres in our model. It can be seen that at low volume fraction, the results of our method are similar with M-G formulas. From $f > 0.4$, the differences become more and more significant. The effect of the material depolarization due to the corners is again visible.

Last, but not least, we consider the general bianisotropic inclusions embedded in a bianisotropic environment. $(\overline{\overline{\varepsilon}}, \overline{\overline{\mu}}, \overline{\overline{\kappa}}_h)$ and $(\overline{\overline{\varepsilon}}, \overline{\overline{\mu}}, \overline{\overline{\kappa}}_i)$ are the relative parameters for the host media and the cubical inclusions, respectively, with

$$\overline{\overline{\varepsilon}} = \overline{\overline{\mu}} = \begin{pmatrix} 10 & 0 & 0 \\ 0 & 10 & 0 \\ 0 & 0 & 5 \end{pmatrix}$$

$$\overline{\overline{\kappa}}_h = \begin{pmatrix} -1 & 0.4 & 0 \\ 0.4 & -0.6 & 0 \\ 0 & 0 & -1.5 \end{pmatrix}$$

and

$$\overline{\overline{\kappa}}_i = \begin{pmatrix} 1 & 0.4 & 0 \\ 0.4 & 0.6 & 0 \\ 0 & 0 & 1.5 \end{pmatrix}.$$

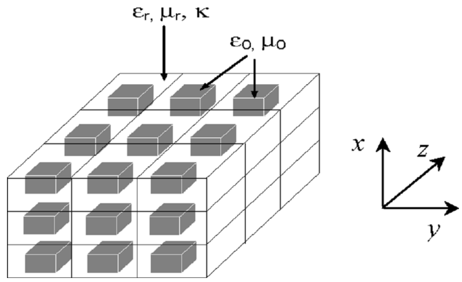

Fig. 9. Finite periodic lattice containing 27 cubical inclusions.

The effective constitutive parameters $\bar{\bar{\varepsilon}}_{\rm eff}$, $\bar{\bar{\mu}}_{\rm eff}$, and $\bar{\bar{\kappa}}_{\rm eff}$ at volume fraction $f_{\max} = 0.512$ are found to be

$$\bar{\bar{\varepsilon}}_{\rm eff} = \bar{\bar{\mu}}_{\rm eff} = \begin{pmatrix} 9.96 & 0 & 0 \\ 0 & 9.98 & 0 \\ 0 & 0 & 4.86 \end{pmatrix}$$

and

$$\bar{\bar{\kappa}}_{\rm eff} = \begin{pmatrix} 0.0223 & 0.399 & 0 \\ 0.399 & 0.0139 & 0 \\ 0 & 0 & 0.0092 \end{pmatrix}.$$

B. Local Field

As a second round of validation of the approach and the numerical codes proposed in this paper, we compare the total electric fields obtained by our method with the results of the classical FEM.

We consider a finite lattice of 27 cells made of chiral material with the parameters $\varepsilon_r = \mu_r = 10$ and $\kappa = 2$ with a vacuum cube located at the center of each cell (Fig. 9). The lattice is truncated by metallic walls, except on the front surface (x–y) where a plane wave with $|E_y| / |E_x| = 2$ is imposed. The electric field is calculated in the central y–z-plane inside the lattice at 10 MHz. The sizes of each vacuum cube and basic cell are 0.125 and 1 cm^3, respectively.

The total electric field can be expressed as

$$E_T = E_T^+ + E_T^- \tag{17}$$

where the signs "+" and "−" correspond to the respective fictional isotropic equivalences in (14).

In each equivalent medium, we perform

$$E_T^\pm = E_{\rm av}^\pm + E_{\rm cor}^\pm \tag{18}$$

where $E_{\rm av}^\pm$ can be obtained by assuming the whole structure is occupied by a homogenized medium with the previously computed effective constitutive parameters, and $E_{\rm cor}^\pm = \nabla_y \Phi^\pm$ can be solved in the unit cell of the lattice.

Fig. 10 represents the amplitude of the x-component of the electric field along the z-axis. In this figure, we plot the averaged $E_{\rm av}$ and corrected fields $E_{\rm cor}$, and then by adding up those two portions, we obtain the total field E_T by (18). For comparative purposes, we also calculate the electric field E by the classical FEM applied to the whole structure, and it is found that good agreement of the results between our method and the classical FEM is achieved. The stability and validity of our improved homogenization method have been confirmed. From this

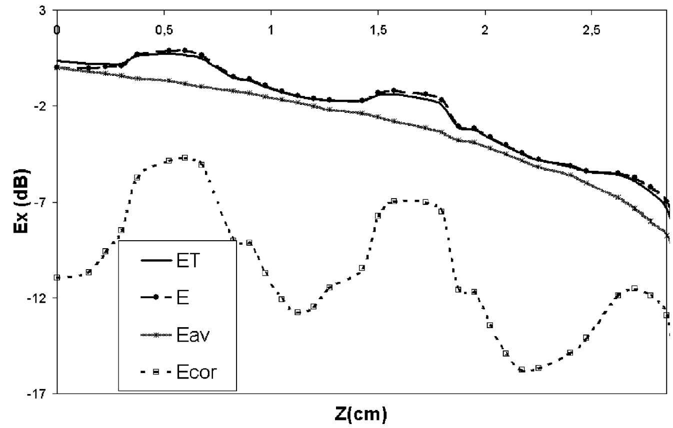

Fig. 10. Magnitude of the x-component of the electric field as a function of position along z-axis at $x = y = L/2$

figure, it can be seen that the averaged field decreases smoothly along the z-direction, while the corrected field varies drastically due to the microscopic heterogeneities, which illustrates the efficiency of the current method compared with the standard homogenization technique (where the field within the microstructure is simply assimilated to averaged field). Therefore, our proposed method provides an effective way to describe the microscopic and macroscopic performances of the composite metamaterials separately and explicitly. It is also shown that only the first-order corrector is required to be taken into account so as to achieve enough good performances.

IV. Conclusion

In this paper, a new asymptotic homogenization approach for 3-D periodic lattices of complex-media inclusions with bianisotropic properties has been proposed. The correctness of our method is verified and the improvement over existing formulas has been shown. The effects of the inclusion shapes and interaction of the edges and corners have been taken into account.

The computed effective parameters along with the corrector fields have been used to estimate, in an accurate manner, the EM fields within finite bianisotropic microstructures with complex-shaped inclusions.

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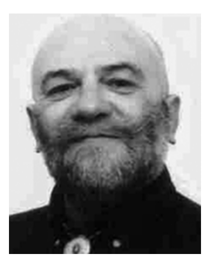

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