An Enhanced Method for Determining Electromagnetic Properties of Periodic Materials

Frederic Lubrano and Frederic Oelhoffen

***Abstract*—A three-dimensional finite-element method with efficient boundary conditions is presented to simulate the electromagnetic properties of heterogeneous periodic materials. The analysis based on a waveguide approach applies to arbitrary profiles with any kind of inclusions for all incidence condition. The Floquet's theorem is used to take into account the periodicity of the problem. This method allows one to handle the scattering effects in the material. For periodically organized composite materials, we can extract an effective permeability and permittivity under certain hypotheses.**

***Index Terms*—Finite-element method (FEM), nonhomogeneous media, periodic structures, permeability, permittivity.**

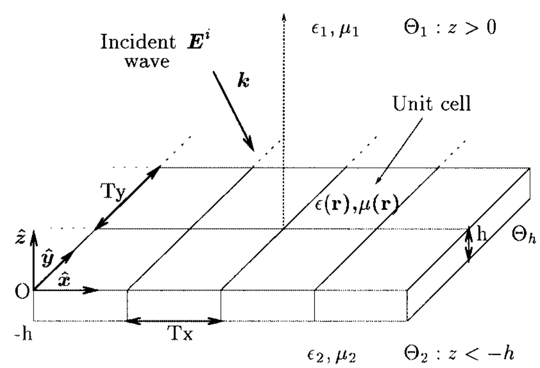

Fig. 1. Schematic representation of a typical case. Tx, Ty stand for the periods of the infinite structure.

I. Introduction

QUASI-STATIC methods are often used to compute the effective permittivity or permeability of periodic (deterministic) heterostructures [1]–[3]. These techniques are restricted to the long-wavelength limit. When the wavelength is shorter than approximately ten periods of the lattice, the homogenization must be performed without assumption in Maxwell's equations.

We report here on a rigorous method capable of computing the complex reflection and transmission coefficients for any periodic composite material of known inclusion characteristics and thickness. The related effective values of permittivity and permeability can then be derived directly as it would be processed from a reflection transmission measurement [4].

A number of techniques have already been applied to analyze the propagation and scattering properties in three-dimensional (3-D) doubly periodic structures. For example, the "coupled-waves" method [5], a finite-difference approach based on a spectral analysis, reduces the 3-D problem to a single variable.

In fact, for highly inhomogeneous media, which can combine magnetic, dielectric, and metallic parts, it is convenient to use a finite-element method (FEM) formulation. The heterogeneity and anisotropy are solved implicitly and rigorously. As part of this approach, the hybrid finite-element/boundary integral methods have been developed to simulate a wide class of complex periodic geometries [6]. This analysis involves the construction of periodic Green's functions.

We propose here a waveguide-oriented technique that takes into account the quasi-periodicity of the fields in the whole space. Our FEM methodology makes use of the 3-D mixed finite elements [7]. Solving the periodic problem requires the definition of new boundary conditions (BCs) on the electromagnetic field: the quasi-periodic BC. For subwavelength periods, only the fundamental mode propagates. The reflection and transmission coefficients computed by the software are introduced in the Weir–Nicholson formula [4] to give the permeability and permittivity of the effective medium. The basic hypothesis of this method is the knowledge of the electromagnetic properties of each inclusion.

II. Boundary-Value Problem

An infinite doubly periodic structure is illuminated by a plane wave (Fig. 1). Assuming an $\exp(i\omega t)$ time dependence, we denote $\boldsymbol{k}(k_x, k_y, k_z)$ as the incident wave vector. The space is separated in three areas: Θ_1, Θ_2 are the homogeneous domains and Θ_h is a domain of thickness h, which includes all the anisotropic inhomogeneities.

The periodicity forces the reflected and transmitted energy to propagate along certain directions. These propagation modes are defined analytically in Θ_1 and Θ_2 by the following.

- $\Delta\boldsymbol{E}^{r,t} + {k_{1,2}}^2\boldsymbol{E}^{r,t} = 0$ with $k_{1,2} = (\epsilon_{1,2}\ \mu_{1,2})^{1/2}\omega$.
- Outgoing waves conditions at $z = \pm\infty$.
- The quasi-periodicity of the fields (periodicity with the phase shift of the oblique incidence wave):

$$\boldsymbol{E}(x + T_x, y + T_y, z) = \mathrm{e}^{-i(k_xT_x + k_yT_y)}\boldsymbol{E}(x, y, z) \quad (1)$$

$$\boldsymbol{H}(x + T_x, y + T_y, z) = \mathrm{e}^{-i(k_xT_x + k_yT_y)}\boldsymbol{H}(x, y, z). \quad (2)$$

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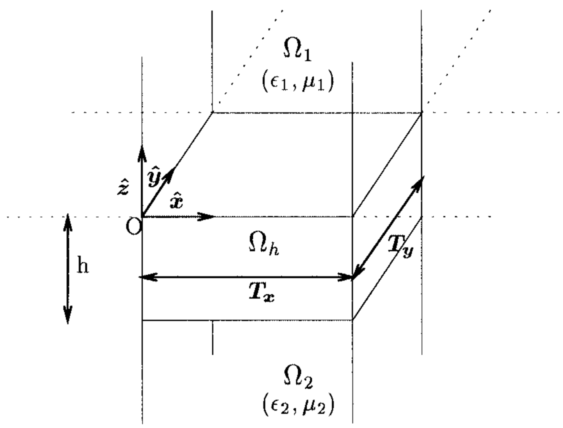

Fig. 2. Finite-element domain: periodic cell.

The scattered field can be expanded on Floquet's modes as

$$\boldsymbol{E} = \boldsymbol{E}^i + \sum_{m,n} \boldsymbol{B}^r_{mn} \mathrm{e}^{-i(\alpha_m x + \beta_n y + \gamma^r_{mn} z)}, \qquad z > 0 \quad (3)$$

$$\boldsymbol{E} = \sum_{m,n} \boldsymbol{B}^t_{mn} \mathrm{e}^{-i(\alpha_m x + \beta_n y - \gamma^t_{mn} z)}, \qquad z < -h \quad (4)$$

and their related wave vectors $\boldsymbol{k}_{mn}$ are determined by

$$\alpha_m = k_x + \frac{2\pi m}{T_x}$$
$$\beta_n = k_y + \frac{2\pi n}{T_y} \quad (5)$$

$$\gamma^{r,t}_{mn} = (k^2_{1,2} - \alpha^2_m - \beta^2_n)^{1/2} \quad (6)$$

$\boldsymbol{B}_{mn}$ are the diffraction coefficients, i.e., the unknowns of our problem. It is worth noting that, for a lossless medium $\Theta_{1,2}$ and when $k^2_{1,2} > (\alpha^2_m + \beta^2_n)$, the (m, n) Floquet's mode propagates (γ_{mn} is real). Otherwise γ_{mn} is purely imaginary and one gets an evanescent wave along z.

Inside the inhomogeneous area Θ_h, the fields satisfy the Bloch conditions (1) and (2). Let us note Ω_h (respectively, $\Omega_{1,2}$) the intersection of Θ_h (respectively, $\Theta_{1,2}$) with the periodic domain $]0, T_x[\times]0, T_y[\times\mathbb{R}$. Ω_h strictly includes all the inhomogeneities. From a numerical point-of-view, we can consider the unit cell Ω_h as a rectangular pseudoguide (Fig. 2) whose sides represent the quasi-periodic conditions for the fields. The input and output modes are Floquet's waves. Thus, we use a waveguide-oriented finite-element approach to handle the periodic problem. Our analysis starts from an FEM technique [8] whose accuracy has been proven for classical waveguide studies.

Let $S^-_x(x = 0)$, $S^+_x(x = Tx)$, $S^-_y(y = 0)$, $S^+_y(y = Ty)$ be the periodic boundaries of the FEM domain Ω_h, and let $S_1(z = 0)$ $S_2(z = -h)$ be its upper and lower face. The solution $\boldsymbol{E}$ of our problem is entirely determined by solving the equations of propagation in Ω_h

$$\nabla \times \left[\mu^{-1}(\boldsymbol{r}) \nabla \times \boldsymbol{E}(\boldsymbol{r})\right] - \epsilon(\boldsymbol{r})\omega^2 \boldsymbol{E}(\boldsymbol{r}) = 0 \quad (7)$$

$$\nabla \cdot \left[\epsilon(\boldsymbol{r})\boldsymbol{E}(\boldsymbol{r})\right] = 0 \quad (\epsilon, \mu \text{ may be tensorial}) \quad (8)$$

with the quasi-periodic BC on tangential components

$$(\boldsymbol{E} \times \hat{\boldsymbol{n}})_{|_{S^+_{x,y}}} = \mathrm{e}^{-ik_{x,y}T_{x,y}} (\boldsymbol{E} \times \hat{\boldsymbol{n}})_{|_{S^-_{x,y}}} \quad (9)$$

$$(\nabla \times \boldsymbol{E}) \times \hat{\boldsymbol{n}}_{|_{S^+_{x,y}}} = \mathrm{e}^{-ik_{x,y}T_{x,y}} (\nabla \times \boldsymbol{E}) \times \hat{\boldsymbol{n}}_{|_{S^-_{x,y}}} \quad (10)$$

and the continuity of total magnetic and electric fields on S_1 and S_2. On these last boundaries, we apply a modal-coupling method, which means we are expanding the fields on Floquet's modes and enforcing the continuity of their tangential components.

III. Mixed Finite-Element Approach

Our FEM software [9] is based on the $H(\mathrm{curl})$ variational formulation. $H(\mathrm{curl}; \Omega)$ is the Sobolev space of summable square vector functions in a bounded regular domain Ω and whose curl square can also be integrated. We use the $P1$ finite-element conforming in $H(\mathrm{curl})$ built on tetrahedron, as introduced by Nedelec [7]. The degrees of freedom are on the edges (i.e., the computed unknown is the line integral of the vector solution along the tetrahedron edge).

The harmonic Maxwell problem is solved in Ω where the propagation equation (7) is discretized by nondivergence polynomial basis functions. A weak formulation of (7) leads to the following problem: find $\boldsymbol{E}$ in $H(\mathrm{curl})$ so that, for all $\boldsymbol{E}'$, we have

$$\int_\Omega \left[-\omega^2 \epsilon(\boldsymbol{E}' \cdot \boldsymbol{E}) + \mu^{-1}(\nabla \times \boldsymbol{E}') \cdot (\nabla \times \boldsymbol{E})\right] dv - \int_S \mu^{-1} \boldsymbol{E}' \cdot \left[(\nabla \times \boldsymbol{E}) \times \hat{\boldsymbol{n}}\right] ds = 0 \quad (11)$$

with S being the boundary of Ω and $\hat{\boldsymbol{n}}$ being its outgoing unit normal vector.

In this FEM, $H(\mathrm{curl})$ is approximated by a finite N-dimensional vectorial space of $P1$ so that we can write an approximation for

$$\boldsymbol{E} = \sum_{i=1}^{N} a_i \boldsymbol{p}_i \quad (12)$$

where the first-order polynomial basis functions $\boldsymbol{p}_i$ have the "mixed-FEM" properties

$$\int_{\Gamma_j} \boldsymbol{p}_i \cdot d\boldsymbol{l} = \delta_{i,j} \quad (13)$$

with Γ_j being the tetrahedron edge and $\delta_{i,j}$ being the Kronecker delta. a_i is the line integral of $\boldsymbol{E}$ along Γ_j. The discretized form of (11) then becomes

$$-\omega^2 MX + KX = G, \qquad \text{with } M_{ij} = \int_\Omega \epsilon \boldsymbol{p}_i \cdot \boldsymbol{p}_j \, dv$$
$$K_{ij} = \int_\Omega \mu^{-1} (\nabla \times \boldsymbol{p}_i) \cdot (\nabla \times \boldsymbol{p}_j) \, dv \quad (14)$$

G_i being the surface term of (11) coming from the sources or Neumann BC or, more generally, from conditions linking the value of the solution to its curl (impedance BC, absorbing

BC, etc.). The factorization of the sparse matrix $(-\omega^2 M + K)$ is performed using a Crout algorithm [10].

IV. Modal-Coupling Method

This technique handles the matching of Floquet's modes on the upper and lower boundary S_1 and S_2 of the domain Ω_h. In order to be a solution of Maxwell's equations in the whole space, tangential components of total magnetic and electric fields must be continuous at these artificial boundaries. We expand the Floquet's modes (3) and (4) on the TE–TM basis where TE and TM is referred, respectively, to the electric- and magnetic-field component normal to the plane of diffraction $(\hat{\boldsymbol{z}}; \boldsymbol{k}_{mn})$. The tangential components of the electric field on S_1 and S_2 can be expressed as

$$\boldsymbol{E}^T(x, y, z) = \sum_{m, n, p} \boldsymbol{E}^T_{mnp}(x, y)\left\{c^+_{mnp}\mathrm{e}^{-i\kappa_{mn}z} + c^-_{mnp}\mathrm{e}^{+i\kappa_{mn}z}\right\} \quad (15)$$

with the convention $\kappa_{mn} = \gamma_{mn}.\overline{n}$ ($\overline{n} = \hat{\boldsymbol{n}}.\hat{\boldsymbol{z}}$), and p being the projection TE ($p = 1$) or TM ($p = 2$). The scalar quantities c^+_{mnp} represent the diffraction coefficients in the TE-TM basis. They are the unknowns of our problem. c^-_{mnp} are the incident data: zero on the lower boundary S_2 (no incident wave) and nonzero on S_1 only for $m = n = 0$ (incident wave). On these surfaces, the TE–TM basis has the form

$$\boldsymbol{E}^T_{mn1}(x, y) = \frac{\mathrm{e}^{-i(\alpha_m x + \beta_n y)}\left(-\beta_n\hat{\boldsymbol{x}} + \alpha_m\hat{\boldsymbol{y}}\right)}{(T_x T_y)^{1/2}\chi_{mn}} \quad (16)$$

$$\boldsymbol{E}^T_{mn2}(x, y) = \frac{\mathrm{e}^{-i(\alpha_m x + \beta_n y)}\left(\alpha_m\hat{\boldsymbol{x}} + \beta_n\hat{\boldsymbol{y}}\right)}{(T_x T_y)^{1/2}\chi_{mn}} \quad (17)$$

with $\chi_{mn} = (\alpha_m^2 + \beta_n^2)^{1/2}$.

The Floquet's modes $\boldsymbol{E}_j$ are characterized by the relation

$$\left[\nabla \times \left(\boldsymbol{E}^{\pm}_j\mathrm{e}^{\mp i\kappa_j z}\right)\right] \times \hat{\boldsymbol{n}}_{|S_{1,2}} = \pm\nu_j\left(\boldsymbol{E}^T_j\mathrm{e}^{\mp i\kappa_j z}\right)_{|S_{1,2}} \quad (18)$$

with $\nu_j = -i\gamma_j$ for TE modes and $\nu_j = \omega^2\epsilon\mu/i\gamma_j$ for TM modes. Therefore, we can write the continuity of tangential components of the total magnetic field on S_1 and S_2 as

$$\left[(\nabla \times \boldsymbol{E}) \times \hat{\boldsymbol{n}}\right]_{|S_{1,2}} = \sum_j Y_j^{(1,2)}\boldsymbol{E}^T_j \quad (19)$$

with

$$Y_j^{(1,2)} = \nu_j(c^+_j\mathrm{e}^{-i\kappa_j z} - c^-_j\mathrm{e}^{+i\kappa_j z})_{|S_{1,2}}. \quad (20)$$

Finally, we express the solution $\boldsymbol{E}$ of the periodic problem in Ω_h as

$$\boldsymbol{E}(\boldsymbol{r}) = \sum_j\left[Y_j^{(1)}\boldsymbol{T}_j^{(1)}(\boldsymbol{r}) + \sum_j Y_j^{(2)}\boldsymbol{T}_j^{(2)}(\boldsymbol{r})\right] \quad (21)$$

where the fields $\boldsymbol{T}_j^{(1)}$ (respectively, $\boldsymbol{T}_j^{(2)}$) are computed in Ω_h by solving, for each mode $\boldsymbol{E}_j$ considered on the boundary S_1 (respectively, S_2), the FEM equation

$$\nabla \times \left[\mu^{-1}(\boldsymbol{r})\nabla \times \boldsymbol{T}_j^{(1,2)}(\boldsymbol{r})\right] - \epsilon(\boldsymbol{r})\omega^2\boldsymbol{T}_j^{(1,2)}(\boldsymbol{r}) = 0 \quad (22)$$

with the modal BC on S_1 and S_2

$$\left(\nabla \times \boldsymbol{T}_j^{(1,2)}\right) \times \hat{\boldsymbol{n}}_{|S_{1,2}} = \boldsymbol{E}^T_j \quad (23)$$

$$\left(\nabla \times \boldsymbol{T}_j^{(1,2)}\right) \times \hat{\boldsymbol{n}}_{|S_{2,1}} = 0 \quad (24)$$

and the quasi-periodic BC on S_x^-, S_x^+, S_y^-, and S_y^+

$$(\boldsymbol{T}_j \times \boldsymbol{n})_{|S^+_{x,y}} = \mathrm{e}^{-ik_{x,y}T_{x,y}}(\boldsymbol{T}_j \times \boldsymbol{n})_{|S^-_{x,y}} \quad (25)$$

$$(\nabla \times \boldsymbol{T}_j) \times \hat{\boldsymbol{n}}_{|S^+_{x,y}} = \mathrm{e}^{-ik_{x,y}T_{x,y}}(\nabla \times \boldsymbol{T}_j) \times \hat{\boldsymbol{n}}_{|S^-_{x,y}}. \quad (26)$$

The modal BCs are the standard Neumann BCs. The nontrivial quasi-periodic BC will be introduced in Section V.

The sum (21) converges to the solution of the problem that we have formulated in Section II. We obtain directly the magnetic field in the cell by applying the curl on (21).

The j sum is, in fact, truncated by choosing a finite number M of Floquet's modes (all the propagating ones and the first vanishing ones). We built the $M \times M$ linear $\{Y_j\}$ system using the continuity on the tangential components of the electric field with (15), (20), and (21). This condition enables us to compute the coefficients of the scattered field expansion, as well as reflection and transmission coefficients.

This method is numerically efficient. It is valid for all frequencies, provided M is chosen large enough.

V. Quasi-Periodic BCs

We are looking for quasi-periodic solutions [see (9) and (10)]. The FEM basis functions (13) should be modified in order that they belong to the solution space (i.e., they must be quasi-periodic). Only basis functions supported on quasi-periodic boundaries will be concerned.

This method requires that the mesh trace is the same on facing boundaries of the cell. Let us note $\{\boldsymbol{p}_k\}_{k=1,N_x}$ is the family of basis functions related to the S_x^- boundary, $\{\boldsymbol{p}_l\}_{l=N_x+1,2N_x}$ are those corresponding to the facing S_x^+ boundary, and $\{\boldsymbol{p}_j\}_{j=2N_x+1,N}$ are all the other ones (the methodology is the same for S_y^- and S_y^+ boundaries). If the mesh is periodic then

$$\boldsymbol{p}_l(\boldsymbol{r})_{|S_x^+} = \boldsymbol{p}_k(\boldsymbol{r})_{|S_x^-}. \quad (27)$$

From (9) and (12), we must have

$$a_l = \mathrm{e}^{-ik_x T_x}a_k. \quad (28)$$

Hence, we built a new set of basis functions $\{\boldsymbol{\Phi}_d\}_{d=1,N-N_x}$

$$\begin{aligned} \boldsymbol{\Phi}_k &= \boldsymbol{p}_k + \mathrm{e}^{-ik_x T_x}\boldsymbol{p}_l, \qquad \text{for } k = [1, N_x]; \\ & \qquad\qquad\qquad\qquad\quad l = [N_x + 1, 2N_x] \\ \boldsymbol{\Phi}_j &= \boldsymbol{p}_{j+N_x}, \qquad \text{for } j = [N_x + 1, N - N_x]. \end{aligned} \quad (29)$$

This new set gives the same properties (13).

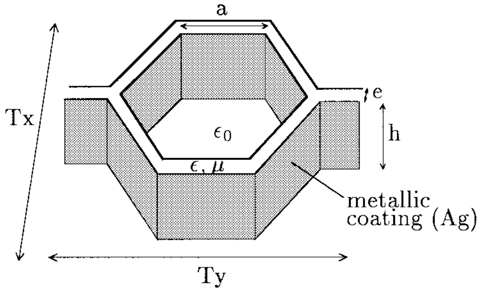

Fig. 3. Honeycomb grid: insulator of permittivity $\epsilon = 3\epsilon_0$ with the vertical faces coated with silver paint of impedance 10 Ω/sq, surrounded by air. The dimensions are $T_x = T_y/\sqrt{3}$, $a = T_y/3$ (hexagonal edge), $e = 0.01T_y$ (insulator gap), and $h = 0.5T_y$ (height).

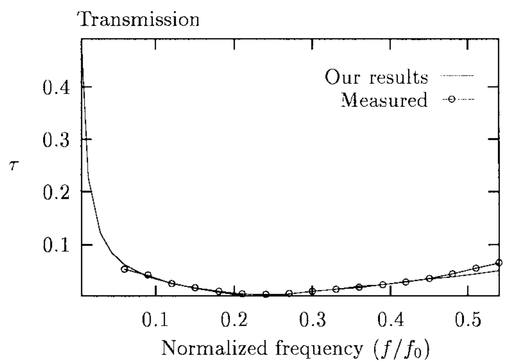

Fig. 4. Computed and measured transmission coefficient (modulus) of the silver honeycomb grid studied. The frequency is normalized to the spatial frequency f_0 given by the largest period T_y: $f_0 = c/T_y$ (diffraction threshold). The incidence is normal ($\boldsymbol{E}^i // \hat{\boldsymbol{y}}$).

Integral (11) is a Hermitian scalar product. The surface term vanishes with the $\{\boldsymbol{\Phi}_d\}$ basis. M and K matrices become Hermitian. The new formulation

$$\boldsymbol{E} = \sum_d a_d \boldsymbol{\Phi}_d \tag{30}$$

enforces the computed electromagnetic field to be quasi-periodic. This method is very easy to handle and leads to a well-formulated FEM for quasi-periodic BCs.

VI. Homogenization of Periodic Materials

We are interested in simulation of periodically organized composite materials. When the periods are small enough compared to the wavelength (i.e., when the scattering can be neglected), the electromagnetic properties of the material can be characterized by an effective permeability μ_e and permittivity ϵ_e. These values are directly obtained from the computed reflection and transmission coefficients [4] that are the measurable quantities. To ensure the homogenization, μ_e and ϵ_e must satisfy a nondependence with the thickness.

The accuracy of the computation of the reflection and transmission coefficients has been proven for several types of frequency-selective surfaces [11]. For a silver honeycomb grid (Fig. 3), we show our results relative to measurements (Fig. 4). The transmission coefficient spectrum is presented for normal incidence. Measurements have been performed on lens-focusing facility [12].

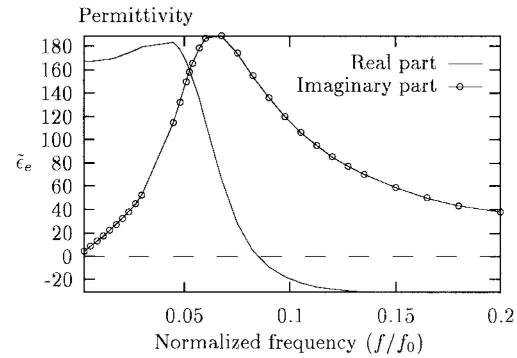

Fig. 5. Effective relative permittivity. $\tilde{\epsilon}_e = (\tilde{\epsilon}_e' - i\tilde{\epsilon}_e'')$.

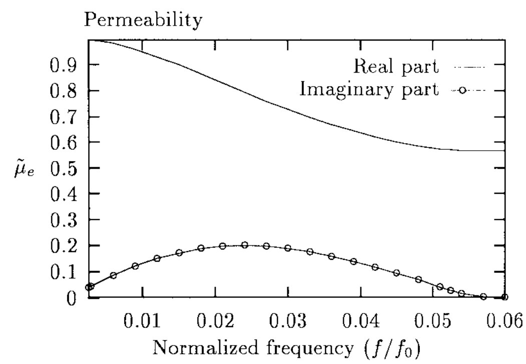

Fig. 6. Effective relative permeability. $\tilde{\mu}_e = (\tilde{\mu}_e' - i\tilde{\mu}_e'')$.

The effective permittivity extracted from the complex transmission and reflection coefficients shows a resonant feature (Fig. 5) usually observed for frequency-selective surfaces. Although the material has no magnetic part, the effective permeability (Fig. 6) varies substantially. $\tilde{\mu}_e'$ is decreasing, while $\tilde{\mu}_e''$ becomes resonant. $\tilde{\mu}_e$ keeps its modulus lower than one. This behavior is related to the skin effect [13]. It is shown that composite materials made of hollow conducting inclusions may exhibit permeability levels significantly different from unity, even for nonmagnetic metal volume fractions lower than 1% [14].

VII. Conclusion

The propagation and diffraction characteristics of any periodic heterostructure can be described rigorously by the present FEM. The scalar coefficients of Floquet's modes and the electromagnetic field in the FEM domain are computed with good accuracy when we consider the first vanishing modes in the calculations. The effective permittivity and permeability of composite materials are then directly derived from the reflection and transmission coefficients.

This method is quite appropriate for the study and design of organized composite dielectrics. Besides, the limit of the homogenization hypothesis can be determined using this software, which is valid for the scattering regime.

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