International Journal of Applied Electromagnetics and Mechanics 18 (2003) 1–4
IOS Press

Low frequency electromagnetic waves in periodic structures

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Abstract. The propagation of electromagnetic waves in three-dimensional periodic structures is studied here using the finite (edge) element method. The use of the Floquet-Bloch theory leads to special boundary conditions. In the quasi-static limit, we obtain the effective properties for a periodic array of dielectric spheres and compare these numerical results with two other homogenization approaches, namely Clausius-Mossotti theory and two-scale method.

Keywords: Bloch conditions, homogenization, photonic crystals

1. Electromagnetic waves in periodic structures

Photonic crystal research has renewed the interest for electromagnetic wave propagation in *periodic structures*. Although real structures are finite and one is often interested in the study of defects, the determination of modes in ideal periodic structures is of foremost importance. The Floquet-Bloch theory reduces the problem to the study of a single cell. The purpose of this paper is to show how to combine this feature with finite element modelling in order to obtain numerical solutions for propagating modes in three-dimensional periodic structures. We draw some numerical comparisons with results gained from the modern theory of homogenization [6] and the original naive approach of Mossotti [9] in the low frequency regime. Our results strengthen those obtained in [1] with a multipole scattering approach.

2. Edge elements and Bloch boundary conditions

The possible formulations are identical to the ones of the resonant cavity problem [3] and as our purpose is to deal not only with dielectric but also with metallic inclusions, the electric field formulation is chosen. According to the Bloch theorem, our problem reduces to looking for Bloch waves solutions which are the solutions $\mathbf{E_k}$ that have the form:

$$\mathbf{E_k}(x,y,z) = e^{i\mathbf{k}\cdot\mathbf{r}}\mathbf{E}(x,y,z) = e^{i(k_x x + k_y y + k_z z)}\mathbf{E}(x,y,z) \tag{1}$$

where $\mathbf{k} = (k_x, k_y, k_z) \in \mathbb{R}^3$ is a parameter (the so-called Bloch vector or quasi-momentum in solid state physics) and $\mathbf{E}(x,y,z)$ is a periodic function on the unit cube $Y =]0;1[^3$.

In order to find Bloch modes with the finite element method, some changes have to be performed with respect to classical boundary value problems that will be named *Bloch conditions* [8,10]. The classical weighted residual is used

$$\mathcal{R}(\mathbf{E_k},\mathbf{E'_k}) = \int_{Y\setminus\bar{\Omega}_m} \mathrm{curl}\,\mathbf{E_k}\cdot\overline{\mathrm{curl}\,\mathbf{E'_k}}\,dxdy - \varepsilon_0\mu_0\omega^2\int_{Y\setminus\bar{\Omega}_m}\varepsilon_r\mathbf{E_k}\cdot\overline{\mathbf{E'_k}}\,dxdy \qquad (2)$$

where Ω_m denotes the area covered by the perfectly conducting inclusion in each basic cell Y. For discretisation, edge elements on a tetrahedral mesh are introduced. The constraint on the mesh is that opposite faces of the cube Y must have exactly the same surface triangular mesh. In the case of a periodic problem, unknowns (i. e. line integrals of $\mathbf{E_k}$) on corresponding edges are imposed to have the same value. In the case of a Bloch problem, equal values up to the phase factor given by (1) are imposed (see figure 1 for illustration in the (x-y) plane). Equations associated to corresponding edges have also to be combined, using the complex conjugate of the phase factor [8,10]. Finally, a generalized eigenvalue problem involving large sparse Hermitian matrices is obtained. The eigenvalues correspond to feasible values of ω^2 for the given Bloch vector $\mathbf{k}$. Such a problem can be solved using a Lanczos algorithm, which permits to compute the largest eigenvalues. Since we are in fact interested in the smallest eigenvalues, the inverse of the matrix of the system must be used in the iterations. The inverse is never computed explicitly but the matrix-vector products are replaced by system solutions thanks to a GMRES method. The practical implementation of the model has been performed thanks to the *GetDP* software [4].

3. Nodal elements and periodic boundary conditions

In this section, we analyse the effective properties of finite photonic crystals of arbitrary shape Ω_f. The theory of homogenization is concerned with the study of the behaviour of solutions of elliptic boundary value problems when the coefficients are periodic with a small period η [2]. The main difficulty in homogenization problems is to pass to the limit in the product of two sequences both of which converge weakly and identify the limit. Due to oscillations, the limit of the product is not equal to the product of the limits, and so this problem is nontrivial. In order to analyze these oscillations in the physical space represented by the macroscopic (or slow) variable $\mathbf{x}=(x,y,z)$, one introduces the so-called microscopic (or fast) variable $\xi=\mathbf{x}/\eta$, and one produces suitable test functions which are then used as multiplier in the original equation. This method of *two-scale convergence* was used in [6] to show that one can homogenize the Maxwell system. The main result of [6] is
When η tends to zero, the solution $\mathbf{E}_\eta$ of a scattering problem $(\mathcal{P}^{\mathbf{E}}_\eta)$ converges weakly in $L^2_{loc}(\mathrm{I\!R}^3)$ to the average of the first term of its asymptotic expansion on the basic cell Y, namely $\mathbf{E}_{hom}(\mathbf{x}) = \int_Y H_0(\mathbf{x},\xi)\,d\xi$, which is the unique solution of the following homogenized problem $(\mathcal{P}^{\mathbf{E}}_{hom})$:

$$(\mathcal{P}^{\mathbf{E}}_{hom}) = \begin{cases} \mathrm{curl}(\mathrm{curl}\,\mathbf{E}_{hom})(\mathbf{x}) - \varepsilon_0\mu_0\omega^2[\varepsilon_{hom}](\mathbf{x})\mathbf{E}_{hom}(\mathbf{x}) = 0 \text{ , in } \Omega_f \\ \mathbf{E}^d_{hom}(\mathbf{x}) = O(\frac{1}{|\mathbf{x}|}) \text{ , in } \mathrm{I\!R}^3\setminus\overline{\Omega_f} \\ \frac{\mathbf{x}}{|\mathbf{x}|}\wedge\mathrm{curl}\,\mathbf{E}^d_{hom}(\mathbf{x}) + ik\mathbf{E}^d_{hom}(\mathbf{x}) = o(\frac{1}{|\mathbf{x}|}) \text{ , in } \mathrm{I\!R}^3\setminus\overline{\Omega_f} \end{cases}$$

where $\mathbf{E}^d_{hom}$ is the diffracted field and $[\varepsilon_{hom}]$ stands for the tensor of homogenized permittivity which is given by

$$[\varepsilon_{hom}](\mathbf{x}) =<\varepsilon_r(\xi)(\mathbf{I}-\nabla_\xi\mathbf{V}_Y(\xi))>_Y \text{ , in } \Omega_f \text{ and } [\varepsilon_{hom}](\mathbf{x}) = \mathbf{I} \text{ , in } \mathrm{I\!R}^3\setminus\overline{\Omega_f}$$

r_c	N_{har}	N_{eff}^{moss}	N_{eff}^{bloc}	N_{eff}^{scal}	N_{ave}
0.1	1.0013992	1.0020952	1.0020968	1.0022840	1.0041801
0.25	1.0225575	1.0329132	1.0332791	1.0374103	1.06343768
0.34	1.0598535	1.0836032	1.0875975	1.0950892	1.1529407
0.43	1.1337499	1.1724446	1.1977349	1.2157954	1.2907658

Table 1

Comparison of effective refractive index N_{eff} given by Clausius-Mossotti's formula (N_{eff}^{moss}), by 'Bloch homogenization' (N_{eff}^{bloc}) and by 'two-scale homogenization' (N_{eff}^{scal}), for different values of the radius r_c of a spherical dielectric inclusion of relative permittivity $\varepsilon_r = 3$ surrounded by air in a cubic unit cell. These values are bounded by the harmonic average $N_{har} = \sqrt{<\varepsilon^{-1}>_Y{}^{-1}}$ and the arithmetic average $N_{ave} = \sqrt{<\varepsilon>_Y}$ (known as scalar wave approximation).

Here, $< f >_Y$ is the average of f in Y (i.e. $\int_Y f(\mathbf{x}, \xi)\ d\xi$). Besides, $\mathbf{V}_Y = (V_1, V_2, V_3)$, where $V_j\ , j \in \{1, 2, 3\}$, is the unique solution in $H^1_\sharp(Y)/\mathbb{R}$ (Hilbert space of Y-periodic square integrable functions with square integrable gradients, defined up to an additive constant) of one of the three following problems $(\mathcal{K}_j)$ of electrostatic type:

$$(\mathcal{K}_j) : \mathrm{div}_\xi \Big[\varepsilon_r(\xi) \big(\nabla_{\mathbf{y}} (V_j(\xi) - \xi_j) \big) \Big] = 0\ , j \in \{1, 2, 3\}\ .$$

Multiplying by V_j in $(\mathcal{K}_j)$, $j \in \{1, 2, 3\}$, and integrating by parts over the basic cell Y leads to the weak formulation (the line integrals cancel out due to periodicity conditions):

$$\Big\langle \varepsilon_r(\xi) \big(\nabla_\xi (V_i - \xi_i) \big) \cdot \nabla_\xi V_j \Big\rangle_Y = 0\ ,\ j \in \{1, 2, 3\}\ .$$

In the discrete formulation the basic cell is meshed with tetrahedra and nodal elements are used for the scalar fields V_j. The GetDP software [4] has been used to set up the finite element problem with some periodicity conditions imposed to the field on opposite sides of the basic cell Y (see [7] for the 2D case).

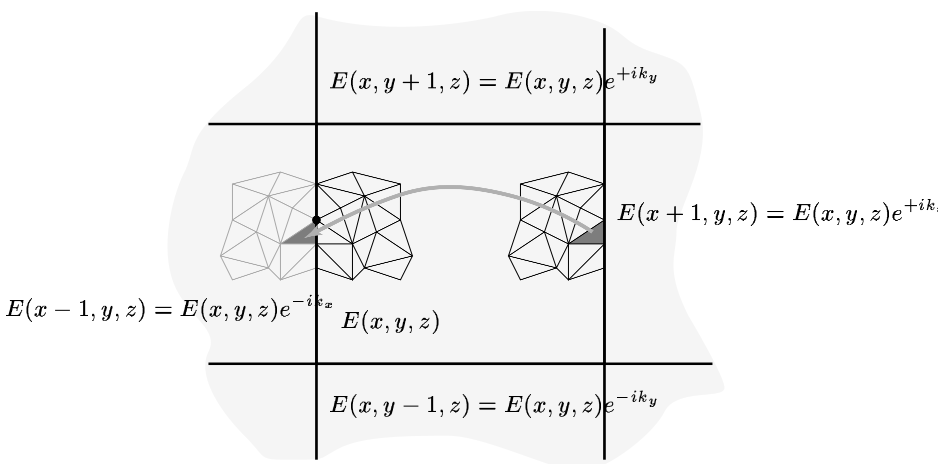

Fig. 1. The Bloch theorem and virtual periodic meshing.

4. Numerical comparisons for three homogenization approaches

Our edge-element formulation for Bloch waves (1) also holds for dielectric inclusions, for this one has just to integrate over the whole cell Y in (2). An interesting issue is then to look at the effective properties of 3D dielectric photonic crystals by means of Bloch approach and to compare it with results given by both two-scale convergence method (see previous section) and the naive approach of Clausius-Mossotti. More precisely, if we consider a dielectric sphere of radius r_c and relative permittivity ε_r surrounded by air in a cubic basic cell $Y =]0;1[^3$, Clausius-Mossotti's formula [9] tells us that the effective refractive index should be $N_{eff}^{moss} = \sqrt{\frac{\varepsilon_r+2f}{\varepsilon_r-f}}$ where $f = \frac{4\pi r_c^3}{3}$ is the volume fraction of the sphere. On the other hand, the effective index N_{eff} can be defined as the limit of $\frac{dk}{d\omega}$ when both the modulus of the Bloch vector k and ω tend to zero (note that in the case of an ellipsoidal inclusion, the previous limit is a tensor since it depends on the trajectory in the coordinates $\{\mathbf{k}, \omega\}$ i.e. the effective material is anisotropic). In our case, if we pick up a point corresponding to a particular Bloch vector in the neighborhood of the origin, say $\mathbf{k} = (\mathbf{0.01}\pi, \mathbf{0}, \mathbf{0})$, the associated lower frequency in the spectrum will provide us with N_{eff}. In the table 1, we report the values for the effective refractive index given by the Mossotti's formula (N_{eff}^{moss}), those provided by edge-element computations for Bloch electromagnetic waves (N_{eff}^{bloc}, see section 2) and nodal-element computations for periodic electrostatic problems (N_{eff}^{scal}, see section 3). Let us also point out that in the 2D case, our results agree well with those of [7]. We should also mention that finite elements were used in [5] for a class of conductive composites exhibiting frequency-dependent effective properties. The homogenization algorithm used by these authors led to vector auxilliary problems solved by means of edge-elements with periodicity conditions on opposite sides of the basic cell Y.

Last, we observe that there is no complete gap for the values of table 1, when $\mathbf{k}_{Bloch}$ describes the Brillouin zone $\Gamma = (0,0,0)$, $X = (0,0,\pi)$, $K = (\pi,\pi,\pi)$ and $M = (\pi,\pi,0)$. Moreover, if we increase the contrast up to $\varepsilon_r = 13$, for a radius $r_c = 0.3$ we found that there is a partial gap running from $\omega \sim 3$ to 3.8 when $\mathbf{k}_{Bloch}$ describes the segment (ΓX) but it shrinks to $\omega \sim 3.6$ at the symmetry point K. This suggests that our structure does not possess filtering properties for all angles and polarisations. Full band diagrams for higher filling fractions of the inclusions would be required to check this conjecture.

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