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Two-scale approach to the homogenization of membrane photonic crystals

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Abstract. Wave propagation and diffraction in a membrane photonic crystal with finite height were studied in the case where the free-space wavelength is large with respect to the period of the structure. The photonic crystals studied are made of materials with anisotropic permittivity and permeability. Use of the concept of two-scale convergence allowed the photonic crystals to be homogenized.

Keywords: homogenization, photonic crystals, metamaterials, effective properties.

1 INTRODUCTION

Photonic crystals, i.e. dielectric or metallic artificial periodic structures, are generally thought of as strongly scattering devices, displaying photonic band gaps. However, their actual electromagnetic behavior when the free-space wavelength is large with respect to the period is also interesting, because it can produce strongly anisotropic behaviors, plasmon frequencies, or even negative index materials [1]. The study of the properties of these structures in this asymptotic regime comes under the theory of homogenization [2–4]. A lot of results are by now well established both for 2D and 3D structures (even for non periodic structures [5–7]).

In this paper, we consider a photonic crystal made of a collection of parallel finite-size fibers embedded in a matrix. This covers the case of structures made out of a layer of bulk materials in which holes are made periodically (membrane photonic crystal) but also the case of structures made out of nanopillars (pillar photonic crystal [8, 9]). The fibers are not supposed to be invariant in the direction of their axis (for instance they can be cone-shaped, see fig. 1). Our point is to derive the effective permittivity and permeability tensors of this structure when the ratio between the period of the structure and the free-space wavelength of the incident field is very small. We had already derived rigorous results for infinitely long cylindrical fibers [3], for which explicit formulas can be derived in some cases [2,10–12]. Here we shall get homogenized permeability and permittivity tensors with a dependence along the axis of the fibers. Let us note that our results hold for dispersive and lossy materials (it applies to imperfect metals as well as to good insulators).

2 TWO-SCALE APPROACH TO HOMOGENIZATION

2.1 Description of the structure and methodology

We consider a 2D photonic crystal such as that in fig. 1. It is constructed from a basic cell \tilde{Y} pictured in fig. 2 ($\tilde{Y} = Y \times (-L, L)$, where $Y = (-1/2, 1/2)^2$). A contraction ratio η is applied to obtain a contracted cell in the horizontal directions ($\tilde{Y}_\eta = \eta^2 Y \times (-L, L)$). In the units of the free-space wavelength, the period of the lattice is thus η . The cells are contained in a cylindrical domain Ω ($\Omega = \mathcal{O} \times (-L, L)$) (cf. fig.1). The domain Ω is thus periodically filled with contracted cells. The space coordinates are denoted by $\mathbf{x} = (x_1, x_2, x_3)$ and we also

Fig. 1. Schematic of the photonic crystal.

denote $\mathbf{x}_{\perp} = (x_1, x_2)$. The coordinates in Y are denoted by $\mathbf{y} = (y_1, y_2)$. We consider time harmonic fields, the time dependence is chosen to be $\exp(-i\omega t)$. For a given monochromatic incident field $(\mathbf{E}^i, \mathbf{H}^i)$, we denote by $(\mathbf{E}^{\eta}, \mathbf{H}^{\eta})$ the total electromagnetic field.

Our aim is to pass to the limit $\eta \to 0$ and determine the limit of the couple $(\mathbf{E}^{\eta}, \mathbf{H}^{\eta})$. In our methodology, we get at the limit a true electromagnetic scattering problem, for a given free-space wavelength λ and a bounded obstacle Ω characterized by some permittivity and permeability tensors. This situation is quite different from other homogenization techniques, making use of periodization conditions, in which the frequency tends to zero, thus not leading to a diffraction problem but rather to an electrostatic one. Such an approach can sometimes give useful explicit formulas but generally leads to complicated formulations [10–12, 20, 21]. Moreover, it does not handle the boundary effects which in some cases may lead to some miscomprehensions [13]. The relative permittivity tensor ϵ^{η} (x) and relative permeability tensor

Fig. 2. Schematic of the basic cell.

 μ^{η} (x) are described by:

$$
\begin{cases} \underline{\underline{\varepsilon}}^{\eta}(\mathbf{x}) = 1, \, \underline{\mu}^{\eta}(\mathbf{x}) = 1 & \text{for } \mathbf{x} \in \mathbb{R}^3 \setminus \Omega \\ \underline{\underline{\varepsilon}}^{\eta}(\mathbf{x}) = \underline{\underline{\varepsilon}}^0(\overline{\frac{\mathbf{x}_\perp}{\eta}}, x_3), \, \underline{\underline{\mu}}^{\eta}(\mathbf{x}) = \underline{\underline{\mu}}^0(\frac{\mathbf{x}_\perp}{\eta}, x_3) & \text{for } \mathbf{x}_\perp \in \Omega \end{cases} \tag{1}
$$

where at fixed x_3 , the applications $y \to \underline{\epsilon}^0 (y, x_3) = (\epsilon_{ij}^0 (y, x_3))$ and $y \to \underline{\mu}^0 (y, x_3) =$ $(\mu_{ij}^0(\mathbf{y},x_3))$ are Y-periodic 3 × 3 matrix functions.

The total electromagnetic field $(\mathbf{E}^{\eta}, \mathbf{H}^{\eta})$ satisfies

$$
\begin{cases}\n\text{curl } \mathbf{E}^{\eta} = i\omega\mu_0 \underline{\mu}^{\eta} \mathbf{H}^{\eta} \\
\text{curl } \mathbf{H}^{\eta} = -i\omega \varepsilon_0 \underline{\varepsilon}^{\eta} \mathbf{E}^{\eta}\n\end{cases}
$$
\n(2)

and $(\mathbf{E}^{s,\eta}, \mathbf{H}^{s,\eta}) = (\mathbf{E}^{\eta} - \mathbf{E}^i, \mathbf{H}^{\eta} - \mathbf{H}^i)$ satisfies Silver-Müller radiation conditions:

$$
\lim_{\|\mathbf{x}\| \to +\infty} \|\mathbf{x}\| \left(Z_0 \mathbf{H}^{s,\eta} \times \frac{\mathbf{x}}{\|\mathbf{x}\|} - \mathbf{E}^{s,\eta} \right) = 0 \tag{3}
$$

where Z_0 is the impedance of vacuum.

2.2 Derivation of the microscopic equations

2.2.1 A short account of the two-scale expansion

In order to describe this problem, we will rely on a two-scale expansion of the fields. That way, the physical problem is described by two variables: a macroscopic one x and a microscopic one y representing the rapid variations of the material at the scale of one basic cell, measured by η . By noticing that there are no rapid variations in the vertical direction x_3 , the microscopic variable is set to be: $y = x_{\perp}/\eta$. Differential operators with respect to variable y are denoted with a subscript y. The fields are periodic with respect to that microscopic variable (this corresponds to the neighborhood of the center of the first Brillouin zone). The limit problem obtained by letting η tend to 0, will then depend on the macroscopic, physical, variable x but also on the microscopic, hidden, variable y. The total limit fields will read $\mathbf{E}^0(\mathbf{x}, \mathbf{y})$ and $\mathbf{H}^0(\mathbf{x}, \mathbf{y})$ and the observable, physical, fields will be given by the mean value over the hidden variable y: $\mathbf{E}(\mathbf{x}) = |Y|^{-1} \int_Y \mathbf{E}^0(\mathbf{x}, \mathbf{y}) d\mathbf{y}$ and $\mathbf{H}(\mathbf{x}) = |Y|^{-1} \int_Y \mathbf{H}^0(\mathbf{x}, \mathbf{y}) d\mathbf{y}$, where |Y| is the measure area of Y . In order to lighten the notations, we denote by brackets the averaging over Y , hence $\mathbf{H}(\mathbf{x}) = \langle \mathbf{H}^0 \rangle$ and $\mathbf{E}(\mathbf{x}) = \langle \mathbf{E}^0 \rangle$.

The main mathematical tool that we use is a mathematically rigorous version of the multiscale expansion, widely used in various areas of physics. More precisely, for a vector field \mathbf{F}^{η} in $(L^2(\Omega))^3$, we say, by definition, that \mathbf{F}^{η} two-scale converges towards \mathbf{F}^0 if for every sufficiently regular function $\phi(\mathbf{x}, \mathbf{y})$, Y-periodic with respect to y, we have:

$$
\int_{\Omega} \mathbf{E}^{\eta}(\mathbf{x}) \cdot \phi(\mathbf{x}, \mathbf{x}_{\perp}/\varepsilon) d\mathbf{x} \to \iint_{\Omega \times Y} \mathbf{E}^{0}(\mathbf{x}, \mathbf{y}) \cdot \phi(\mathbf{x}, \mathbf{y}) d\mathbf{x} d\mathbf{y},
$$
\n(4)

as η tends to 0.

The limit field \mathbf{F}^0 is square integrable with respect to both variables x and y and is Yperiodic in the y variable (this is the definition of the space $L^2\left(\Omega;\left(L_{per}^2(Y)\right)^3\right)$). A complete analysis of this new mathematical tool can be found in [14].

We make the physically reasonable assumption that the electromagnetic energy remains bounded when η tends to 0, which is equivalent to assume that $(\mathbf{E}^{\eta}, \mathbf{H}^{\eta})$ are both locally square integrable. Then it is known [14] that $(\mathbf{E}^{\eta}, \mathbf{H}^{\eta})$ two-scale converges towards limit fields $(\mathbf{E}^0, \mathbf{H}^0)$. This physical assumption could be justified mathematically, however it seems quite obvious, from the point of view of physics, that the limit fields exist. The point is then to give the system of equations that is satisfied by these fields and to derive the effective permittivity and permeability tensors.

2.2.2 The equations at the microscopic scale

First of all, we have to determine the set of equations that are microscopically satisfied, that is, satisfied with respect to the hidden variable y, for that will give the constitutive relations of the homogenized medium. Multiplying Maxwell-Faraday equation by a regular test function $\phi\left(\mathbf{x}, \frac{\mathbf{x}_\perp}{n}\right)$ η), and integrating over Ω , we obtain:

$$
\int_{\Omega} \mathbf{E}^{\eta}(\mathbf{x}) \cdot \left[\operatorname{curl}_{x} (\phi) + \frac{1}{\eta} \operatorname{curl}_{y} (\phi) \right] d\mathbf{x} = i\omega \mu_{0} \int_{\Omega} \underline{\mu}^{\eta}(\mathbf{x}) \mathbf{H}^{\eta}(\mathbf{x}) \phi(\mathbf{x}, \mathbf{x}_{\perp}/\eta) d\mathbf{x}.
$$
 (5)

Multiplying by η and letting η tend to 0, we get using (4):

$$
\iint_{\Omega \times Y} \mathbf{E}^{0} \left(\mathbf{x}, \mathbf{y} \right) \cdot \operatorname{curl}_{y} \left(\phi \right) d\mathbf{x} d\mathbf{y} = 0. \tag{6}
$$

This is equivalent to:

$$
\iint_{\Omega \times Y} \operatorname{curl}_y \mathbf{E}^0(\mathbf{x}, \mathbf{y}) \cdot \phi(\mathbf{x}, \mathbf{y}) d\mathbf{x} d\mathbf{y} = 0 \tag{7}
$$

which is nothing else but the variational form for: curl_y $\mathbf{E}^0 = 0$. In a very similar way, but using now Maxwell-Ampere equation, we get curl $y\mathbf{H}^0 = 0$. On the other hand, since $\underline{\varepsilon}^{\eta} \mathbf{E}^{\eta}$ is divergence free, we have, for every test function $\phi(\mathbf{x}, \mathbf{y}), \int_{\Omega} \underline{\varepsilon}^{\eta}(\mathbf{x}) \mathbf{E}^{\eta}(\mathbf{x}) \cdot \left[\nabla_x \phi + \frac{1}{\eta} \right]$ $\frac{1}{\eta} \nabla_y \phi \, d\mathbf{x} = 0.$ Multiplying by η and letting η tend to 0, we get:

$$
\iint_{\Omega \times Y} \underline{\varepsilon}^{0} \left(\mathbf{y}, x_{3} \right) \mathbf{E}^{0} \left(\mathbf{x}, \mathbf{y} \right) \cdot \nabla_{y} \phi \, d\mathbf{x} d\mathbf{y} = 0, \tag{8}
$$

which can be written as (notice that the div_y operator acts only on the transverse components):

$$
\operatorname{div}_y \left(\underline{\varepsilon}^0 \mathbf{E}^0 \right) = 0. \tag{9}
$$

Similarly, since the magnetic field is divergence free, we derive:

$$
\operatorname{div}_y \left(\underline{\mu}^0 \mathbf{H}^0 \right) = 0. \tag{10}
$$

Summing up, we have the following microscopic equations, holding inside the basic cell Y :

$$
\begin{cases} \operatorname{div}_{y} \left(\underline{\mu}^{0} \mathbf{H}^{0} \right) = 0 \\ \operatorname{curl}_{y} \overline{\mathbf{H}}^{0} = 0 \end{cases}, \begin{cases} \operatorname{div}_{y} \left(\underline{\varepsilon}^{0} \mathbf{E}^{0} \right) = 0 \\ \operatorname{curl}_{y} \overline{\mathbf{E}}^{0} = 0 \end{cases}
$$
\n(11)

2.3 Derivation of the homogenized parameters

The systems in (11) are respectively of electrostatic and magnetostatic types. This means that, with respect to the hidden variable y, the electric field and magnetic field satisfy the static Maxwell system. This property is true only at that scale and not at the macroscopic scale. However, it is these static equations that determine the effective permittivity and permeability. Indeed let us analyze this system starting with the electric field. From the curl relation, we get $\nabla_y E_3^0 = 0$, and so $E_3^0(\mathbf{x}, \mathbf{y}) \equiv E_3(\mathbf{x})$. Besides, the basic cell having the geometry of a flat torus, we get the existence of a regular periodic function $w_E(\mathbf{y})$ such that:

$$
\mathbf{E}_{\perp}^{0} = \mathbf{E}_{\perp} + \nabla_{y} w_{E}. \tag{12}
$$

The function w_E is the electrostatic potential associated with the microscopic electrostatic problem. Inserting (9) in equation (12) and projecting on both horizontal axis, we obtain:

$$
\text{div}_y \left[\underline{\underline{\varepsilon}}^0 \right] \left(\mathbf{e}_i + \nabla_y w_{E,i} \right) = 0, \ i \in \{1, 2\} \tag{13}
$$

where $\underline{\varepsilon}^0$ denotes the 2 × 2 matrix extracted from \leq by removing the last line and last column. By linearity, denoting $\mathbf{E}_{\perp} = (E_1, E_2)$, we derive that the potential w_E is given by $w_E = E_1 w_{E,1} + E_2 w_{E,2}$, where $w_{E,i}$ are the periodic solutions of (13). We stress that these potentials depend upon y but also on x_3 . In fact, we get a family of homogenization problems parametrized by the vertical coordinate. By (12) we obtain:

$$
\mathbf{E}^{0}\left(\mathbf{x},\mathbf{y}\right)=\mathcal{E}\left(\mathbf{y},x_{3}\right)\mathbf{E}\left(\mathbf{x}\right)
$$
\n(14)

where:

$$
\mathcal{E}(\mathbf{y}, x_3) = \begin{pmatrix} 1 + \partial_{y_1} w_{E,1} & \partial_{y_1} w_{E,2} & 0 \\ \partial_{y_2} w_{E,1} & 1 + \partial_{y_2} w_{E,2} & 0 \\ 0 & 0 & 1 \end{pmatrix}
$$
(15)

The magnetic field H^0 can be handled in the same way since it satisfies exactly the same kind of equations as H^0 (see (11)). In particular, we may represent its tranversal component in the form: $\mathbf{H}_{\perp}^0 = \mathbf{H}_{\perp} + \nabla_{\perp} w_H$, where w_H is a periodic magnetic potential (the possibility of this representation is due to the curl-free condition which means that no microscopic current is present). Analogously as in (14,15), we find:

$$
\mathbf{H}^{0}\left(\mathbf{x},\mathbf{y}\right) = \mathcal{M}\left(\mathbf{y},x_{3}\right)\mathbf{H}\left(\mathbf{x}\right) \tag{16}
$$

where

$$
\mathcal{M}\left(\mathbf{y}\right) = \left(\begin{array}{ccc} 1 + \partial_{y_1} w_{H,1} & \partial_{y_1} w_{H,2} & 0\\ \partial_{y_2} w_{H,1} & 1 + \partial_{y_2} w_{H,2} & 0\\ 0 & 0 & 1 \end{array}\right) \tag{17}
$$

where:

$$
\text{div}_y \left[\underline{\mu}^0 \right] (\mathbf{e}_i + \nabla_y w_{H,i}) \right] = 0, \ i \in \{1, 2\}
$$
 (18)

and μ^0 denotes the 2 × 2 matrix extracted from μ^0 by removing the last line and last column. Of course, the same remark as in the case of electric potentials holds: the functions $w_{H,i}$ depend on the vertical coordinate x_3 . The above results show that, at the microscopic scale, the limit fields $(\mathbf{E}^0, \mathbf{H}^0)$ are completely determined by the physical fields (\mathbf{E}, \mathbf{H}) . Now that the microscopic behavior is precised, we are able to determine the macroscopic system satisfied by (E, H) . To that aim, let us choose a regular test function $\phi(\mathbf{x})$ independent of variable y. From Maxwell equations we get

$$
\begin{cases}\n\int_{\Omega} \mathbf{H}^{\eta}(\mathbf{x}) \cdot \operatorname{curl}(\phi) d\mathbf{x} = -i\omega \varepsilon_{0} \int_{\Omega} \underline{\varepsilon}^{\eta}(\mathbf{x}) \mathbf{E}^{\eta}(\mathbf{x}) \phi(\mathbf{x}) d\mathbf{x} \\
\int_{\Omega} \mathbf{E}^{\eta}(\mathbf{x}) \cdot \operatorname{curl}(\phi) d\mathbf{x} = i\omega \mu_{0} \int_{\Omega} \underline{\mu}^{\eta}(\mathbf{x}) \mathbf{H}^{\eta}(\mathbf{x}) \phi(\mathbf{x}) d\mathbf{x}\n\end{cases}
$$
\n(19)

passing to the limit $\eta \rightarrow 0$, we get:

$$
\begin{cases}\n\iint_{\Omega \times Y} \mathbf{H}^{0}(\mathbf{x}, \mathbf{y}) \cdot \operatorname{curl}(\phi) d\mathbf{x} d\mathbf{y} = -i\omega \varepsilon_{0} \iint_{\Omega \times Y} \underline{\varepsilon}^{0}(\mathbf{y}, x_{3}) \mathbf{E}^{0}(\mathbf{x}, \mathbf{y}) \phi(\mathbf{x}) d\mathbf{x} d\mathbf{y} \\
\iint_{\Omega \times Y} \mathbf{E}^{0}(\mathbf{x}, \mathbf{y}) \cdot \operatorname{curl}(\phi) d\mathbf{x} d\mathbf{y} = i\omega \mu_{0} \iint_{\Omega \times Y} \underline{\mu}^{0}(\mathbf{y}, x_{3}) \mathbf{H}^{0}(\mathbf{x}, \mathbf{y}) \phi(\mathbf{x}) d\mathbf{x} d\mathbf{y}\n\end{cases}
$$
\n(20)

Recalling that $\langle \mathbf{E}^0 \rangle = \mathbf{E}$ and that $\langle \mathbf{H}^0 \rangle = \mathbf{H}$, we get:

$$
\begin{cases}\n\operatorname{curl} \mathbf{E} = i\omega\mu_0 \left\langle \underline{\mu}^0 \mathbf{H}^0 \right\rangle \\
\operatorname{curl} \mathbf{H} = -i\omega\varepsilon_0 \overline{\left\langle \underline{\varepsilon}^0 \mathbf{E}^0 \right\rangle}\n\end{cases}
$$
\n(21)

which, taking into account $(14,16)$, brings to the limit system:

$$
\begin{cases}\n\operatorname{curl} \mathbf{E} = i\omega\mu_0 \left\langle \underline{\mu}^0 \mathcal{M} \right\rangle (x_3) \mathbf{H} \\
\operatorname{curl} \mathbf{H} = -i\omega\varepsilon_0 \overline{\left\langle \underline{\varepsilon}^0 \mathcal{E} \right\rangle (x_3)} \mathbf{E}\n\end{cases}
$$
\n(22)

2.3.1 The special case of a 1D grating

Let us specialize the above results to the case of a one dimensional grating (fig. 3) that is, the pillars are invariant in the x_2 and x_3 directions (the basic cell Y is depicted in fig. 3). We assume also that the pillars are made on a non-magnetic material and that the relative permittivity tensor is given by:

$$
\underline{\underline{\varepsilon}}^{0}(y_{1}) = \begin{pmatrix} \varepsilon_{1}(y_{1}) & 0 & 0\\ 0 & \varepsilon_{2}(y_{1}) & 0\\ 0 & 0 & \varepsilon_{3}(y_{1}) \end{pmatrix}
$$
(23)

Fig. 3. Schematic of the 1D photonic crystal. The inset shows the basic cell Y .

The invariance of $\underline{\varepsilon}^0$ with respect to y_2 and the periodicity condition suggest that we look for solutions that are y₂-independent. Let us first consider $w_{E,2}$ which satisfies: $\partial_{y_1} (\varepsilon_1 \partial_{y_1} w_{E,2}) = 0$. This implies that $w_{E,2} = \text{cste}$. Next, we turn to $w_{E,1}$. It satisfies: $\partial_{y_1} [\varepsilon_1 (1 + \partial_{y_1} w_{E,1})] = 0$ Therefore $\varepsilon_1 (1 + \partial_{y_1} w_{E,1}) = \text{cste} = C$. Let us now average this relation, we get: $C \left(\frac{1}{\varepsilon_1} \right)$ ε_1 $\rangle =$ $\langle 1 + \partial_{y_1} w_{E,1} \rangle$. Due to the periodicity of $w_{E,1}$, we have: $\langle \partial_{y_1} w_{E,1} \rangle = 0$ and finally: $C =$ $/1$ ε_1 $\sum_{n=1}^{\infty}$. The homogenized relative permittivity tensor is given by:

$$
\langle \underline{\varepsilon}^0 \mathcal{E} \rangle = \begin{pmatrix} \left\langle \frac{1}{\varepsilon_1} \right\rangle^{-1} & 0 & 0\\ 0 & \langle \varepsilon_2 \rangle & 0\\ 0 & 0 & \langle \varepsilon_3 \rangle \end{pmatrix}
$$
(24)

We retrieve a well-established result concerning the homogenization of 1D photonic crystals [2].

3 DISCUSSION

The homogenized permeability and permittivity tensors are respectively $\langle \mu^0 \mathcal{M} \rangle$ and $\langle \underline{\varepsilon}^0 \mathcal{E} \rangle$. Both are matrix functions of the coordinate x_3 . In case of cylindrical fibers (i.e. invariant along their axis), we would find that the effective tensors coincide with that obtained in the polarized cases [2, 3, 15]. In fact, because the permittivity and permeability tensors are not renormalized with respect to η , the homogenization process is purely local, that is, the effective constitutive relations are local ones. However, we emphasize that the locality is lost if we change the scale of the permittivity or permeability coefficients in the obstacles. In particular, the results obtained in the case of infinite conductivities in the polarized case [3] cannot be transposed to the case of fibers with finite length, due to the emergence of surprising non local effects which are studied in [16–18]. In this context, another problem is interesting: it is the study of the situation where the height L of the pillar is small with respect to the free-space wavelength. An ansymptotic study can be performed in that case, leading to a simplified formulation of the diffraction problem [19].

We also note that an approach relying on explicit calculations, for instance using Blochwaves theory or Fourier-Bessel expansions, cannot work here, due the lack of an explicit representation of the fields in case of finite size fibers. The method that is used here proves to be particularly efficient, the results are obtained at the cost of very few calculations. Besides, it gives an interesting physical pictures of the homogenization process in terms of hidden variables: the homogenized parameters are obtained through clearly defined electrostatic and magnetostatic problems with respect to these variables. It should also be noted that the case of dielectric materials with losses is handled by our result. This result can be straightforwardly applied to the study of membrane photonic crystal in the low frequency range where phenomena of birefringence and dichroism are obtained [20, 21].

In our homogenization result, it is clear that the main numerical problem is the solving of the annex problems (13,18) for they give the effective matrices $\mathcal E$ and $\mathcal M$. In certain simple cases, for instance that of circular isotropic non magnetic rods and a permittivity constant in each connected region, it is possible to find an explicit expression for the effective permittivity (it is in fact a very old problem). However, for more complicated geometries, there is a general numerical procedure based on fictitious sources, that allows to solve both annex problems at a low numerical cost. It should also be stressed that if the wavelength is not very large with respect to the period, the device may still be homogenizable, but then the evanescent fields play an important role [22] that can make the effective parameters be dependent upon the environnement of the device.

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