Metasurfaces homogenization technique based on the computation of the average value of the contravariant tensors elements

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Abstract. The purpose of this paper is to present a 2D metasurfaces homogenization based on the computation of the average value of the contravariant tensors elements. A simple semi-analytical model for the comprehension of the extraordinary optical transmission (EOT) through a 2D array of periodic subwavelength metasurface is analyzed through the proposed method. In this single mode model, the mono layer of the metasurface film is considered as homogeneous medium. Therefore, the electromagnetic response of this structure to a plane wave excitation is equivalent to that of a slab with homogeneous equivalent properties. In a coordinates system where the coordinate curves \( x_j \) coincide with the physical discontinuity of the material, the covariant formalism involving contravariant components of density flux and covariant components of the electromagnetic field, allows to efficiently handle the continuity properties of the electromagnetic field. By averaging all these quantities involving local fields over the periods of the unit cell, and assuming that, these macroscopic fields and densities satisfy a constitutive relationship, the electromagnetic parameters such as averaged permittivity and permeability can be defined.

1. Introduction
A simple semi-analytical model for the comprehension of the extraordinary optical transmission (EOT) [1, 2, 3] through a 2D array of periodic subwavelength metasurface is analyzed. In this single mode model, the mono layer of the metal film is considered as homogeneous medium. Therefore, the electromagnetic response of this structure to a plane wave excitation is equivalent to that of a slab with homogeneous equivalent permittivity. Typically, this problem involves several kinds of coordinates systems. Indeed, the elementary rectangular cell introduces a Cartesian coordinate system while the profile of the elementary pattern may be better described with some specific curvilinear coordinate system following its contour. It is then useful to define a change of coordinates that continuously transforms one coordinate curve to the other. The covariant formalism of Maxwell’s equations will be the starting point of the works presented in this paper. This formalism provides the following two advantages:

- the covariant components of the electromagnetic field \( E_k \) and \( H_k \) are continuous through any coordinate surfaces \( x^j = \text{cste} \ (j \neq k) \),
- the contravariant components of electric density flux \( D^j \) and magnetic density flux \( B^j \) are continuous through the coordinate surfaces \( x^j = \text{cste} \),
Consequently, in an arbitrary coordinates system where the coordinate curves \( x^j \) coincide with borders delimiting physical discontinuity of the material, the covariant formalism involving contravariant components of density flux and covariant components of the electromagnetic field, allows to efficiently handle the continuity properties of the electromagnetic field. Averaging all these quantities allows to define macroscopic electromagnetic parameters such as averaged permittivity and permeability.

2. Constitutive relations in covariant formalisme and homogenization technique

Consider the 3D vector space with the natural basis \((e_1, e_2, e_3)\) associated with the curvilinear coordinates system \((x^1, x^2, x^3)\). At any point \(X(x^1, x^2, x^3)\), the density vectors components \(D^i\), \(B^i\) and the electromagnetic field components \(E_k, H_k\) are simply linked through the constitutive relations:

\[
D^i = \varepsilon^{ij}E_j = \varepsilon g^{ij}E_j, \quad B^i = \mu^{ij}H_j = \mu g^{ij}H_j,
\]

where \(\varepsilon^{ij}\), (resp. \(\mu^{ij}\)) denotes the contravariant permittivity (resp. permeability) tensor of the medium that depends on both physical properties of the medium and the metric of the coordinate system \((x^i)\). \(g_{ij}\) are the covariant components of the metric tensor of the coordinate system \((x^j)\). Scalar functions \(\varepsilon\) and \(\mu\) generally depend on the variables \(x^1\) and \(x^2\). To illustrate our homogenization technique based on the tensors elements averaging, let us first consider a simple case of an isotropic metric tensor \(\sqrt{g}g^{ij} = \sqrt{g}\delta_{ij}\). From the constitutive relations, it follows for \(E_1, E_2,\) and \(D^3\) components

\[
\begin{bmatrix}
E_1 \\
E_2 \\
D^3
\end{bmatrix}
= 
\begin{bmatrix}
1/\varepsilon^{11}(x^1, x^2) & 0 & 0 \\
0 & 1/\varepsilon^{22}(x^1, x^2) & 0 \\
0 & 0 & \varepsilon^{33}(x^1, x^2)
\end{bmatrix}
\begin{bmatrix}
D^1 \\
D^2 \\
D^3
\end{bmatrix}.
\]

At the scale of the period, the electromagnetic field can be assumed to be constant. Therefore, the electromagnetic field quantities, namely normal components of electric density flux and tangential components of electric field, that are continuous at the interfaces defined by the coordinates surfaces \(x^1 = \text{constant}\) and \(x^2 = \text{constant}\), can be supposed to be constant. Consequently

\[
\begin{align*}
\langle E_1(x^1, x^2) \rangle &= \langle 1/\varepsilon^{11}(x^1, x^2)D^1(x^1, x^2) \rangle = \langle 1/\varepsilon^{11} \rangle D^1 \\
\langle E_2(x^1, x^2) \rangle &= \langle 1/\varepsilon^{22}(x^1, x^2)D^2(x^1, x^2) \rangle = \langle 1/\varepsilon^{22} \rangle D^2, \\
\langle D^3(x^1, x^2) \rangle &= \langle \varepsilon^{33}(x^1, x^2)E_3(x^1, x^2) \rangle = \langle \varepsilon^{33} \rangle E_3
\end{align*}
\]

where \(\langle \phi(x^1, x^2) \rangle\) denotes the averaged value of the quantity \(\phi\) over the periodic unit cell. The averaged permittivity associated with the equivalent effective medium is defined throughout the following relation:

\[
\begin{bmatrix}
\langle D^1 \rangle \\
\langle D^2 \rangle \\
\langle D^3 \rangle
\end{bmatrix}
= 
\begin{bmatrix}
1/\varepsilon^{11} & 0 & 0 \\
0 & 1/\varepsilon^{22} & 0 \\
0 & 0 & \varepsilon^{33}
\end{bmatrix}
\begin{bmatrix}
\langle E_1 \rangle \\
\langle E_2 \rangle \\
\langle E_3 \rangle
\end{bmatrix}.
\]

In a suited coordinates system allowing to handle efficiently boundary conditions, the metric tensor turns out to be dependent not only on the direction of propagation, but also on the geometry of the scatters encapsulated in the unit cell. Therefore, the homogenized quantities namely the permittivity and the permeability tensors efficiently take into account not only all physical boundary conditions and the average characteristics of the periodic structure but also the geometrical details of the periodic structure. The matched coordinates system \([4, 5, 6]\) is a specific curvilinear coordinates system that continuously transforms one coordinate curve to the
other. In this coordinates system, the coordinate surfaces \( x^j = \text{constante} \) are defined in order to match the inclusions (nano resonators) shape to the unit cell border. See Fig. (1). From the constitutive relation in the matched coordinates, we can write:

\[
\begin{bmatrix}
E_1 \\
E_2 \\
D^3
\end{bmatrix} =
\begin{bmatrix}
\tilde{\varepsilon}^{11}(x^1, x^2) & \tilde{\varepsilon}^{12}(x^1, x^2) & 0 \\
\tilde{\varepsilon}^{21}(x^1, x^2) & \tilde{\varepsilon}^{22}(x^1, x^2) & 0 \\
0 & 0 & \varepsilon^{33}(x^1, x^2)
\end{bmatrix}
\begin{bmatrix}
D_1^1 \\
D_2^2 \\
E_3^3
\end{bmatrix}.
\] (4)

A sufficient condition for the continuity of the normal component \( D_n \) at the scatter boundary, is that the contravariant components of the densities \( D_1 \) and \( D_2 \) are continuous on the coordinate surfaces \( x^j = \text{constante} \). Therefore by averaging equations Eq.(4), the explicit form of the permeability (and/or permittivity) tensor of the equivalent homogeneous medium can be defined. Because of the matched coordinates system, the homogenized material parameters is expected to be consistent enough with other properties of the medium, such as the geometric details of the inclusions within a unit cell and also the arrangement of the resonators. By using a single mode model described in references [7, 8, 9] with a suitable phase correction, we can provide an analytical expression of the transmission \( T \) of the structure:

\[
T = \frac{t_1 t_2 s_1 e^{-ik_0 \gamma h}}{1 + r_1 e^{-ik_0 \gamma h} s_1 r_2 s_3 e^{-ik_0 \gamma h}}
\] (5)

where \( t_i \) and \( r_i \) are the Fresnel coefficients of the upper and downer interfaces. See Fig. (2). The parameters \( s_i \) hold the coupling between the cavity mode \( \gamma \) and the interfaces plasmon modes. We compare the spectrum of the transmission Fig. (3) of the structure obtained with the single mode model to those obtained from a rigorous method, namely the polynomial modal method PMM [10, 11]. The results are clearly close to those of the PMM simulations. This homogeneous equivalent slab model clearly provides the resonance frequency of the extraordinary transmission mechanism. However, the result provided by the approximate model is higher than the rigorous
Figure 3. Left side: spectrum of the $\gamma$-mode. Right side: Comparison between the transmission computed with polynomial modal method and the approximate model.

numerical simulation. This is undoubtedly due to the fact that only a not less important part of the incident energy is conveyed by the mode of the structure. As it is shown on Fig. (3), by judiciously weighting the transmission $T$ of Eq. (5), the analytical model fits well the rigorous computation.

**Funding**

This work has been sponsored by the French government research program "Investissements d’Avenir" through the IDEX-ISITE initiative 16-IDEX-0001 (CAP 20-25)

**References**

[1] T.W. Ebbesen, H.J. Lezec, H.F. Ghaemi, T. Thio and P.A. Wolff, "Extraordinary optical transmission through sub-wavelength hole arrays," Nature, 391, 667–669 (1998).

[2] L. Martin-Moreno, F.J. Garcia-Vidal, H.J. Lezec, K.M. Pellier, T. Thio, J.B. Pendry and T.W. Ebbesen, "Theory of Extraordinary Optical Transmission through Subwavelength Hole Arrays," Phys. Rev. Lett., 86, 1114–1117 (2001).

[3] F. J. Garcia de Abajo, R. Gomez-Medina, and J. J. Saenz, "Full transmission through perfect-conductor subwavelength hole arrays," Phys. Rev. E., 72, 016608 (2005).

[4] T. Weiss, G. Granet, N. A. Gippius, S. G. Tikhodeev, and H. Giessen, "Matched coordinates and adaptive spatial resolution in the Fourier modal method," Optics Express 17, 8051-8061 (2009).

[5] S. Essig, K. Busch, "Generation of adaptive coordinates and their use in the Fourier Modal Method", Optics Express 18, 8051-8061 (2010).

[6] K. Edee, and J.-P. Plumey, A. Moreau and B. Guizal, "Matched coordinates in the framework of polynomial modal methods for complex metasurfaces modeling," J. of Opt. Soc. of Am. A, 35, 608–615 (2018).

[7] K. Edee, "Single mode approach with versatile surface wave phase correction for the extraordinary optical transmission comprehension of 1D period nano-slits arrays," Opt. Soc. of Am. Cont., 1, 613–624 (2018).

[8] K. Edee, "Understanding the plane wave excitation of the metal-insulator-metal gap plasmon mode of a nanoribbons periodic array: role of insulator-metal-insulator lattice mode," Opt. Soc. of Am. Cont., 2, 389–399 (2019).

[9] K. Edee, M. Benrouma, M. Antezza, J. A. Fan, B. Guizal, "Coupling between subwavelength nano-slit lattice modes and metal-insulator-graphene cavity modes: a semi-analytical model," Opt. Soc. of Am. Cont., 2, 1296–1309 (2019).

[10] K. Edee, "Modal method based on subsectional Gegenbauer polynomial expansion for lamellar gratings," J. of Opt. Soc. of Am. A, 28, 2006–2013 (2011).

[11] K. Edee, and J.-P. Plumey, "Numerical scheme for the modal method based on subsectional Gegenbauer polynomial expansion: application to biperiodic binary grating," J. of Opt. Soc. of Am. A, 32, 402–410 (2015).