Accuracy of effective medium parameter extraction procedures for optical metamaterials

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An effective medium parameter extraction procedure that incorporates first-order spatial dispersion effects is devised to study the homogenization of a one-dimensional stack. It is shown that for such a stack, the proposed extraction procedure yields effective medium parameters that characterize the medium with improved accuracy and are independent of the number of unit cells composing the stack. It is also shown that in the optical regime, where it is difficult to realize a unit cell of a width that is much smaller than the wavelength, the inaccuracy due to use of an extraction procedure that assumes no spatial dispersion can be prohibitively high. This work establishes the importance of extending the common extraction procedure so as to account for spatial dispersion contributions.

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The use of metamaterials to create artificial homogeneous substances with useful properties in the optical regime has gained enormous popularity in recent years.[1–5] However, a recent increase in studies that report unusual or unexpected results whose physical origin is unclear has led to some skepticism regarding the validity of the homogenization approaches employed.[6–8] Of special concern is the large number of studies that describe simulation and experimental results in the optical regime obtained using a thickness of only a small number of unit cells, commonly only one. Also, a substantial body of work involves the extraction of homogenized parameters for structures where the unit cell dimension is too large compared to the excitation wavelength. While these choices are understandable considering the difficulties inherent in nanoscale growth processes, as a consequence, the extracted homogenized parameters may be rendered meaningless.

This paper describes an effective medium parameter extraction procedure that incorporates first-order correction terms stemming from first-order spatial dispersion. Every medium that is not truly homogeneous exhibits spatial dispersion, meaning that the polarization and magnetization at a specific point in space are dependent not only on the fields values at that point, but also on their spatial variation. The order of the spatial dispersion corresponds to the number of Taylor series terms that are accounted for in the representation of the spatial relation between both the polarization and magnetization and the fields. Use of the proposed extraction procedure is important for a valid estimation of the error introduced by realizing a desired artificial homogeneous substance with a given metamaterial. The extraction procedure can also be used with higher order correction terms to obtain an equivalent medium that, while generally being dependent on incidence angle, is superior in terms of accuracy. To simplify the new extraction procedure, we assume that the metamaterial is a one-dimensional (1D) stack of homogeneous layers. This assumption reduces the number of extracted effective medium parameters when incorporating first-order spatial dispersion contributions, and allows a simple interpretation of these terms as originating from asymmetry with respect to flipping the stack around the surface normal. This work also reveals that for a 1D stack, the first-order correction terms are independent of the number of unit cells composing the stack. While results for a 1D stack serve the purpose of evaluating the error introduced by using a simple finite metamaterial to realize an artificial homogeneous substance in the optical regime, the derivation of the extraction procedure also lays the foundations for more complicated parameter extraction procedures suitable for general three-dimensional metamaterials.

A 1D stack can be considered as having fourfold symmetry about the stack axis, and two symmetry planes parallel to this symmetry axis (see Fig. 1). These symmetries make the stack a member of the $4mm$ symmetry class, having uniaxial omega medium constitutive relations.[9] When z is the stack axis and the temporal dependency is $e^{-i\omega t}$, the constitutive relations are given by

$$\mathbf{D} = \bar{\bar{\epsilon}} \cdot \mathbf{E} + i\sqrt{\epsilon_0\mu_0}\bar{\bar{\kappa}} \cdot \mathbf{H}, \tag{1}$$

$$\mathbf{B} = \bar{\bar{\mu}} \cdot \mathbf{H} - i\sqrt{\epsilon_0\mu_0}\bar{\bar{\kappa}}^T \cdot \mathbf{E}, \tag{2}$$

where $\mathbf{E}$ and $\mathbf{H}$ are the electric and magnetic fields, respectively, $\mathbf{D}$ and $\mathbf{B}$ are the electric and magnetic flux densities, respectively,

$$\bar{\bar{\epsilon}} = \epsilon_0 \begin{bmatrix} \epsilon_t & 0 & 0 \\ 0 & \epsilon_t & 0 \\ 0 & 0 & \epsilon_n \end{bmatrix}, \quad \bar{\bar{\mu}} = \mu_0 \begin{bmatrix} \mu_t & 0 & 0 \\ 0 & \mu_t & 0 \\ 0 & 0 & \mu_n \end{bmatrix}, \tag{3}$$

$$\bar{\bar{\kappa}} = \begin{bmatrix} 0 & K & 0 \\ -K & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix},$$

are the effective permittivity, permeability, and chirality dyadics, respectively, and ϵ_0 and μ_0 are the free space permittivity and permeability, respectively. Note that not all metamaterials have symmetry properties that allow first-order spatial dispersion effects of the type yielding a nonchiral chirality dyadic as in Eq. (3). Using the expressions for the reflection and transmission coefficients in uniaxial omega slabs,[10] it is possible to relate the scattering matrix elements measured for a plane wave impinging on the stack to the effective material parameters. For TE polarized inci-

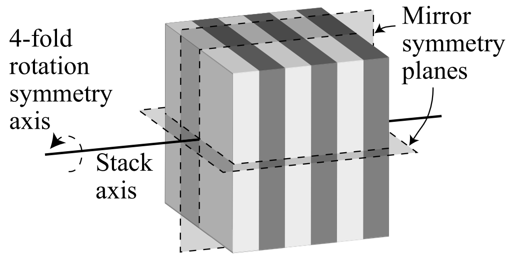

FIG. 1. Symmetries of a 1D stack configuration used for determination of the constitutive relations.

dence at an angle θ relative to the stack axis, these relations are given by

$$\mu_{\mathrm{TE},t} = \frac{[(1+S_{11})(1+S_{22}) - S_{12}^2]\beta}{k_0 \cos\theta\sqrt{[(1-\sqrt{S_{11}S_{22}})^2 - S_{12}^2][(1+\sqrt{S_{11}S_{22}})^2 - S_{12}^2]}}, \tag{4}$$

$$\epsilon_{\mathrm{TE},t} - \frac{\sin^2\theta}{\mu_{\mathrm{TE},n}} = \frac{[(1-S_{11})(1-S_{22}) - S_{12}^2]\beta\cos\theta}{k_0\sqrt{[(1-\sqrt{S_{11}S_{22}})^2 - S_{12}^2][(1+\sqrt{S_{11}S_{22}})^2 - S_{12}^2]}}, \tag{5}$$

$$K_{\mathrm{TE}} = \frac{i(S_{11}-S_{22})\beta}{k_0\sqrt{[(1-\sqrt{S_{11}S_{22}})^2 - S_{12}^2][(1+\sqrt{S_{11}S_{22}})^2 - S_{12}^2]}}, \tag{6}$$

where S_{ij} are the elements of the scattering matrix, $k_0 = \omega\sqrt{\epsilon_0\mu_0}$ is the free space wave number, and β is the propagation constant in the z direction, given for both polarizations by

$$\beta = \frac{1}{L}\arccos\left[\frac{1-(S_{11}S_{22}-S_{12}^2)}{2S_{12}}\right]. \tag{7}$$

Here, L is the thickness of the stack. In case of uncertainty, the branch of the multivalued functions $\sqrt{(\cdot)}$ and $\arccos(\cdot)$ in Eqs. (4)–(7) should be chosen based on causality and continuity of the solutions with respect to frequency.[11] Corresponding relations for the TM polarization can be obtained via duality.

Both the proposed extraction procedure (PEP) and the common extraction procedure[12] (CEP) begin with a configuration-specific calculation or measurement of the scattering matrix elements. However, the procedures differ in the way those scattering matrix elements are used to calculate the effective medium parameters. The CEP does not account for first-order spatial dispersion, and thus assumes that the elements of the chirality dyadic [$\bar{\bar{\kappa}}$ in Eqs. (1) and (2)] are zero. Consequently, the CEP uses a simplified set of equations that implicitly assume symmetry ($S_{11}=S_{22}$) to extract only ϵ and μ out of a reduced set of scattering matrix elements. The PEP, on the other hand, does take first-order spatial dispersion effects into account. This is done by substituting the full set of scattering matrix elements into Eqs. (4)–(6), which were derived specifically for the uniaxial omega medium representing the homogenized stack. Note that once the stack becomes symmetric ($S_{11}=S_{22}$), K_{TE} in Eq. (6) becomes zero, and the other extracted material parameters in Eqs. (4) and (5) coincide with those obtained by the CEP. However, many common metamaterial structures do not possess this type of symmetry.

Rewriting the expressions in Eqs. (4) and (6) using elements of the unit cell translation matrix T, which relates the complex amplitudes of the incident and reflected fields in one layer of a unit cell to those of the equivalent layer in the next unit cell, we have

$$\mu_{\mathrm{TE},t} = \frac{[(T_{11}-T_{22})+(T_{12}-T_{21})]\beta}{2ik_0\cos\theta\sqrt{1-[(T_{11}+T_{22})/2]^2}}, \tag{8}$$

$$\epsilon_{\mathrm{TE},t} - \frac{\sin^2\theta}{\mu_{\mathrm{TE},n}} = \frac{[(T_{11}-T_{22})-(T_{12}-T_{21})]\beta\cos\theta}{2ik_0\sqrt{1-[(T_{11}+T_{22})/2]^2}}, \tag{9}$$

$$K_{\mathrm{TE}} = \frac{(T_{21}+T_{12})\beta}{2k_0\sqrt{1-[(T_{11}+T_{22})/2]^2}}. \tag{10}$$

In order to obtain an analytic expression for the translation matrix of N cascaded stacks, we use Abeles' matrix method (assuming reciprocity of the stack components),[13] which results in

$$T^N = \begin{pmatrix} T_{11}U_{N-1}(\tilde{T}) - U_{N-2}(\tilde{T}) & T_{12}U_{N-1}(\tilde{T}) \\ T_{21}U_{N-1}(\tilde{T}) & T_{22}U_{N-1}(\tilde{T}) - U_{N-2}(\tilde{T}) \end{pmatrix}, \tag{11}$$

where

$$U_{N-1}(\tilde{T}) = \frac{\sin[N\arccos(\tilde{T})]}{\sqrt{1-\tilde{T}^2}} \quad \text{and} \quad \tilde{T} = \frac{T_{11}+T_{22}}{2}. \tag{12}$$

Replacing the elements of T in Eqs. (8)–(10) with the expressions for the elements of T^N, it can be easily shown that the extracted material parameters are independent of N in the 1D case we study. The fact that the extracted material parameters of a given unit cell in a finite one-dimensional periodic stack do not change when re-extracting them from a cascaded set of the same unit cell is important for a meaningful definition of effective medium. However, this property does not apply to extracted material parameters obtained via the CEP for a stack with an asymmetric unit cell.[14]

To demonstrate the PEP, we study the effective medium parameters obtained by applying it [determining, in this case analytically, the scattering matrix elements and substituting them in Eqs. (4)–(6)] to the simple finite periodic stack shown in Fig. 2. The stack is composed of two alternating dielectric slabs and can be divided into unit cells that can be asymmetric (see Fig. 2). For TE polarized incidence at an angle θ relative to the stack axis, the first terms in the Taylor expansion of the material parameters about the normalized unit cell thickness $k_0 d=0$ are given by

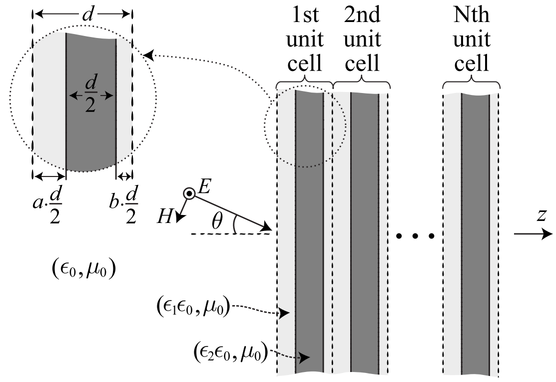

FIG. 2. Properties of the configuration studied. The 1D stack is illuminated by a TE plane-wave.

$$\mu_{\mathrm{TE},t} = \mu_{\mathrm{TE},n} = 1 - \left\{ \frac{[1-(a-b)^2]\Delta\epsilon}{32} \right\} k_0^2 d^2 + O(k_0^3 d^3), \tag{13}$$

$$\epsilon_{\mathrm{TE},t} = \bar{\epsilon} - \left\{ \frac{\{[1+3(a-b)^2]\epsilon_1 - 4\bar{\epsilon}\}\Delta\epsilon}{96} \right\} k_0^2 d^2 + O(k_0^3 d^3), \tag{14}$$

$$K_{\mathrm{TE}} = \left\{ \frac{(a-b)\Delta\epsilon}{8} \right\} k_0 d + O(k_0^3 d^3), \tag{15}$$

where d is the stack's unit cell thickness, $\Delta\epsilon = \epsilon_2 - \epsilon_1$, $\bar{\epsilon} = (\epsilon_1 + \epsilon_2)/2$, and ϵ_1 and ϵ_2 are the relative dielectric constants of the alternating dielectric slabs. Also, a and b correspond to the normalized thicknesses of the two dielectric slabs at the left and right sides of the unit cell, respectively (see Fig. 2). The thicknesses a and b are normalized to half the unit cell dimension, yielding the relation $a+b=1$. In what follows, material parameters of a certain order of approximation are calculated considering terms in Eqs. (13)–(15) only up to that order in $k_0 d$. The three lowest order approximations can be interpreted as stemming from the inclusion of zero, first, and second order spatial dispersion effects, respectively. As is evident in Eq. (13), terms corresponding to second-order spatial dispersion effects or higher can induce artificial magnetic properties in the effective medium representation.[9] Note in Eqs. (13)–(15) that all higher order terms in the expressions for the material parameters are proportional to the contrast between the dielectric constants of the alternating dielectric slabs. This supports the general assumption that the accuracy of an effective medium representation of a metamaterial is decreased with an increase in the scattering strength of inclusions within the metamaterial unit cell. Note also that the incidence angle θ does not affect the extracted material parameters up to the second order terms in $k_0 d$. Therefore, for TE incidence, material parameters of a higher order of approximation that were obtained via the procedure proposed above can be used as a more accurate general effective medium. For TM incidence, however, the incidence angle θ does affect the higher order extracted material parameters, and thus, an incidence angle dependent equivalent medium should be used to describe the stack. While being more accurate, such a description holds only for the planar stack of Fig. 2, which has infinite transverse dimension.

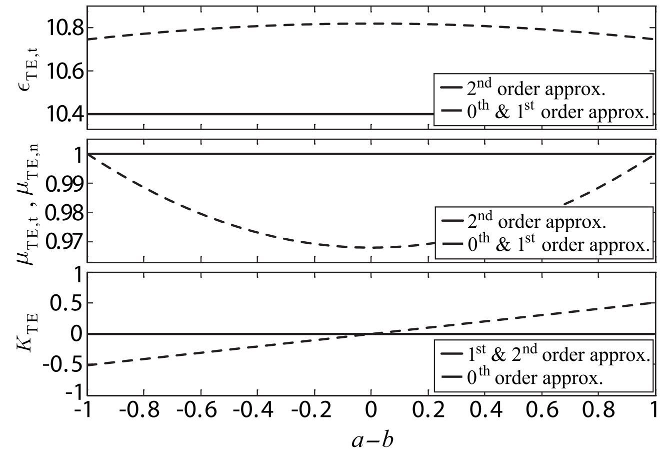

FIG. 3. First and second order approximations for the material parameters [obtained using Eqs. (13)–(15)] vs $(a-b)$, representing the asymmetry of the unit cell for $d/\lambda_0 = 0.04$, $\epsilon_1 = 2.3$, and $\epsilon_2 = 18.5$.

Figure 3 shows the effect of the stack asymmetry on the extracted material parameters for a SiO_2-Si stack in air. While the zeroth order approximation of the material parameters can also be obtained via the CEP, a valid first- and second-order approximation can only be obtained using the extraction procedure suggested above. Note in Fig. 3 that plots of the first- and second-order approximation of the extracted parameters are clearly dependent on the asymmetry of the stack's unit cell. Figure 4 shows the range of unit cell thicknesses for which the different order approximations of the material parameters of the SiO_2-Si stack hold for green light (free space wavelength of $\lambda_0 = 500$ nm). It is evident from Fig. 4 that for this midrange optical wavelength, a second-order approximation of the material parameters is

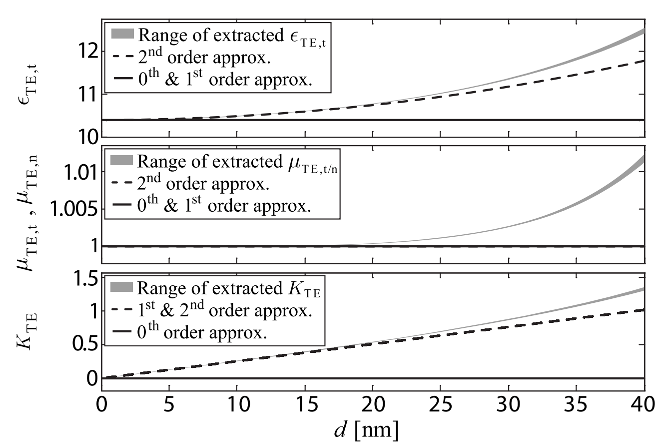

FIG. 4. Extracted material parameters [obtained using Eqs. (13)–(15)] vs the thickness of the unit cell d for $a-b=1$, $\epsilon_1 = 2.3$, $\epsilon_2 = 18.5$, and $\lambda_0 = 500$ nm. The gray area corresponds to fully extracted parameters [from Eqs. (4)–(6)] for all possible incident angles assuming that $\mu_{\mathrm{TE},n} = \mu_{\mathrm{TE},t}$.

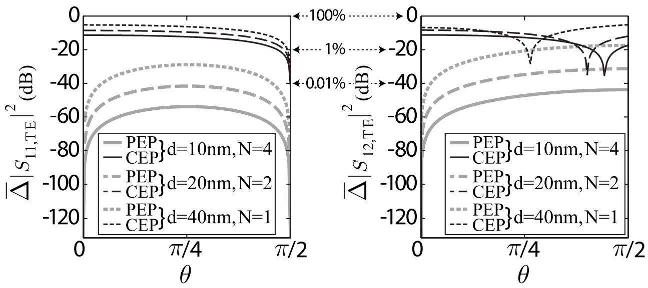

FIG. 5. Normalized error in the reflectivity ($\bar{\Delta}|S_{11,TE}|^2$) and transmissivity ($\bar{\Delta}|S_{12,TE}|^2$) of the stack, as these are approximated using effective medium parameters obtained via the PEP (depicted by thick gray curves) and the CEP (depicted by thin dark curves). The errors are normalized with respect to exact values of the reflectivity and transmissivity (obtained here via analytic solution of scattering by the stack) and are plotted vs the incident angle θ for $a-b=1$, $\epsilon_1=2.3$, $\epsilon_2=18.5$, and $\lambda_0=500$ nm. Different plots correspond to stacks with different unit cell thicknesses (d) and different number of unit cells (N).

necessary for an accurate description of stacks with a unit cell thickness larger than $d=20$ nm. Manufacturing stacks with smaller unit cell thicknesses may be prohibitively difficult due to restrictions on the accuracy of growth processes that affect the planarity of the stack as the number of comprising layers increases. This indicates that using the CEP to evaluate material parameters of currently manufacturable stacks in the optical regime may result in inaccurate values.

To determine the merits of the PEP, we examine the accuracy with which the effective medium parameters extracted via the PEP predict the reflectivity and transmissivity of a given stack, and compare the results with those obtained using effective medium parameters extracted via the CEP. To this end, Fig. 5 shows the normalized error in the reflectivity and transmissivity of the stack, as these are approximated using effective medium parameters obtained via the PEP and the CEP. Both extraction procedures use scattering matrix elements of a simulated measurement (obtained here via analytical solution of scattering by the stack) at normal incident angle. The PEP uses those scattering matrix elements in Eqs. (4)–(6) for the extraction, assuming that $\mu_{\mathrm{TE},n}=\mu_{\mathrm{TE},t}$. Note that, from Eqs. (13)–(15), the PEP holds as long as $(k_0 d)^3 \ll 1$, while the CEP holds only when $k_0 d \ll 1$, where the relative effective permeability is unity due to the use of nonmagnetic materials. We therefore *a priori* assume in the CEP that the relative effective permeability is $\mu=1$ and employ the common extraction formula $\mu/\epsilon=[(1+S_{11}^2)^2-S_{12}^2]/[(1-S_{11}^2)^2-S_{12}^2]$ (see Ref. 12) to extract the relative effective permittivity ϵ. The relative effective permittivity can be also extracted using $\mu\epsilon=\{\arccos\{[1-(S_{11}S_{22}-S_{12}^2)]/2S_{12}\}/k_0 d\}^2$ (see Ref. 12), however the multivalued nature of the $\arccos(\cdot)$ function makes it more complicated and less likely to be used with a physical measurement. It is evident from Fig. 5 that for TE polarized green light ($\lambda_0=500$ nm) impinging on a SiO_2-Si stack with unit cell thicknesses between 10 and 40 nm, the PEP substantially improves the prediction of measurable quantities such as the reflectivity and transmissivity.

This work constitutes the first step toward studying metamaterials using improved effective medium extraction procedures that take first-order spatial dispersion contributions into account. The suggested extraction procedure for 1D stacks fully incorporates the asymmetric nature of the stacks into the extracted effective material parameters, allowing a true estimation of the accuracy of the effective medium approximation of finite sized stacks. The simplified 1D stack example shows that the suggested corrections to the zeroth order effective medium approximation are important for an accurate prediction of the capabilities of devices in the optical regime.

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