Thickness conditions for characterizing the periodic nanostructures with the retrieved electromagnetic parameters

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By analyzing the convergence of the retrieved effective electromagnetic parameters, we presented that one wavelength of the propagating wave in the nanostructure is the minimum thickness requirement for effectively characterizing a finite thickness nanostructure. This thickness condition has been separately validated in a photonic crystal with negative refraction and in a typical fishnet metamaterial which has been investigated theoretically and experimentally before.
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Keywords: Photonic crystal, retrieved electromagnetic parameters, negative refraction

1 INTRODUCTION

Periodic nanostructures, such as photonic crystals (PCs) and metamaterials, are often characterized by the effective electromagnetic parameters based on implicit assumptions inspired by natural material models [1]. In most cases, these effective electromagnetic parameters are obtained by utilizing the field averaging [2]–[6], extended Maxwell-Garnett [7]–[10] or S-parameter retrieval method [11]–[20]. However, different from bulk homogeneous material, the retrieved parameters of nanostructures, especially the fishnet metamaterials, are always sensitive to the slab thicknesses [21]–[24]. Therefore, in this respect, most experimental samples such as the stacking of three-functional [25], four-functional [26], and ten-functional [27, 28] layers and even the thickest fabricated fishnet structures cannot be treated as a homogeneous metamaterial with effective electromagnetic parameters.

Although we have known that these parameters will be converged and independent of the slab thicknesses when the slab thickness increases to some extent [21]–[24], it is still unclear what is the minimum thickness prerequisite for achieving this convergence and what is the underlying physics. In this paper, we focus on tackling these problems. Unlike the works on the convergence of retrieved parameters in fishnet metamaterials, we take a PC with a negative refractive index as an example, and systematically investigate the dependence of the retrieved effective electromagnetic parameters on the distances between the input/output port and the PC slab. Nevertheless, we will borrow the similar phenomena discussed intensively in fishnet metamaterials to analyze the physics underlying the thickness conditions. Particularly, we will establish guidelines for the thickness conditions under which the periodic nanostructures such as PCs and metamaterials can be characterized by the effective electromagnetic parameters.

2 MODEL AND METHOD

The two-dimensional (2D) dielectric PC slab with a negative refractive index we take as an example is shown in Figure 1(a). This PC structure is made of a square lattice of air holes etched in a low loss material with dielectric permittivity constant $\varepsilon = 10.6$ [29]. The lattice constant is a and the diameter of the air hole is $2r = 0.7a$. Throughout this paper we only consider the transverse-magnetic (TM) modes whose electric field is polarized along the air holes.

Using the plane wave expansion method, the band structure of this PC is calculated and shown in Figure 1(b), where the frequency (f_{nor}) is normalized to a/λ_0 (λ_0 is the wavelength in vacuum). As shown in Figure 1(b), a left-handed dispersion branch can be noted in the second band. The normalized fre-

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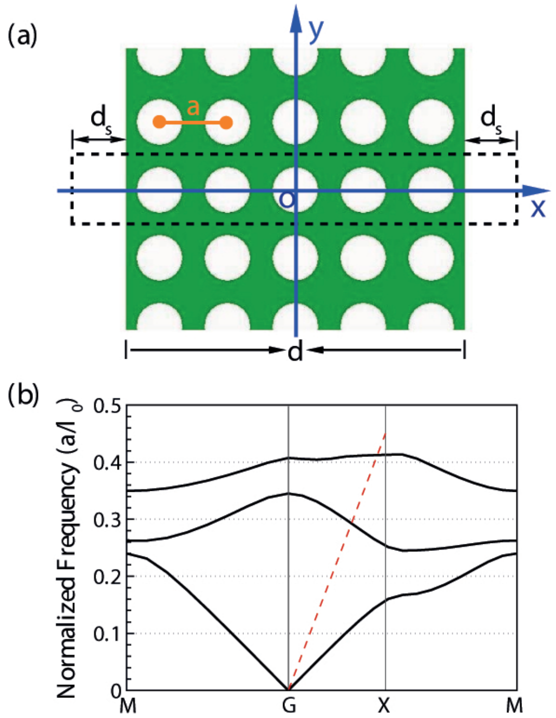

FIG. 1 (a) Schematic of the PC and the coordinate system describing simulation processes. (b) Band structure of the PC for the TM polarization. The dashed line denotes the light line in vacuum.

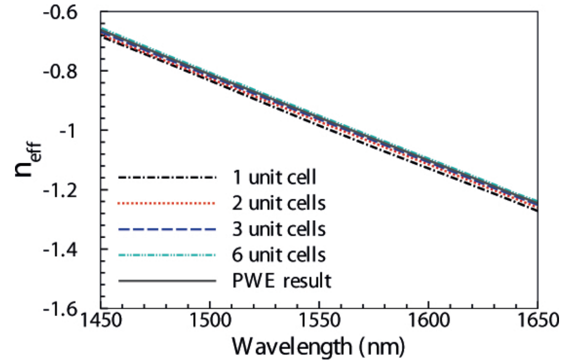

FIG. 2 Retrieved effective refractive index $n_{\rm eff}$ with d_s = 0 nm for different number of unit cells.

quency $f_{\rm nor}$ = 0.2858, at which the effective index $n_{\rm eff} = -1$, is denoted by the intersection point between the light line and the second band along the Γ-X direction. With a = 443 nm, this normalized frequency corresponds to the telecommunication wavelength λ = 1550 nm.

Although the PCs are beyond the traditional long wavelength limit [8], they can be described by the effective parameters under the single-mode approximation [30, 31]. For electromagnetic waves incident normally to the PC surfaces, the effective refractive index $n_{\rm eff}$ and effective impedance $z_{\rm eff}$ are related to the reflection coefficient S_{11} at the front interface and the transmission coefficient S_{21} at the back interface by [11]

$$n_{\rm eff} = \frac{1}{k_0 d}\arccos\left[\frac{1}{2S_{21}}(1 - S_{11}^2 + S_{21}^2)\right] + \frac{2m\pi}{k_0 d}, \qquad (1)$$

$$z_{\rm eff} = \pm\sqrt{\frac{(1+S_{11})^2 - S_{21}^2}{(1-S_{11})^2 - S_{21}^2}}, \qquad (2)$$

where m is an integer related to the branch index of the real part of effective refractive index Re($n_{\rm eff}$), d is the slab thickness, and k_0 is the wave number of the incident wave in free space. Since the PC is a passive medium, the corresponding real part of effective impedance Re($z_{\rm eff}$) and imaginary part of effective refractive index Im($n_{\rm eff}$) must be greater than zero according to the causality. This retrieval procedure is initially presented by Weir [32], and now has been successfully applied to periodic nanostructures [11]–[20].

The transmission and reflection coefficients, used in the retrieval procedure, are obtained by using the finite-difference time-domain (FDTD) method [33] in this paper. Periodic boundary conditions are employed to simulate an infinite lattice perpendicular to the direction of propagation, and perfectly matched layers are used for the remaining boundaries. Along the propagation direction, two recorders are located at at d_s away from the PC interfaces to record S'_{11} and S'_{21}, respectively. Then, the S parameters at the slab interfaces, which are used in the retrieval procedure, can be obtained by $S_{11} = S'_{11}\exp(-ik_0 2d_s)$ and $S_{21} = S'_{21}\exp(-ik_0 2d_s)$. With this kind of configuration, the finite-thickness nanostructures cannot be treated as a homogeneous material if the retrieved parameters are dependent on either d_s or the thicknesses.

3 RESULTS AND DISCUSSION

To check these dependence of our photonic crystal samples, we first calculated the effective refractive index $n_{\rm eff}$ as a function of wavelength λ for one unit cell, two, three and six unit cells of PC with d_s = 0 nm. For comparison, the $n_{\rm eff}$ of the infinite PC has also been figured out by solving the master equation using the plane wave expansion (PWE) method. As shown in Figure 2, all curves of the $n_{\rm eff}$ almost overlapped each other and the $n_{\rm eff}$ increases monotonously with λ from about −1.25 to −0.65. These results indicated that for all retrieved models with d_s = 0 nm, irrespective of the numbers of unit cells, mimic very closely the infinite periodic nanostructure. Just for this reason, this configuration with d_s = 0 nm has been widely used for electromagnetic characterizing the infinite nanostructures. However, most of the fabricated samples at optical wavelengths were only a few layers. Are the effective parameters of the infinite nanostructures still suitable for such thin samples?

In fact, there are complicated surface waves generated at the interfaces between the periodic nanostructure and the free space. For a very thin nanostructure, the surface waves at the front interface always extend to the back one. As a result, the retrieved effective electromagnetic parameters will vary with d_s till the effects of the surface waves can be ignored.

To avoid the effects of the surface waves, we adopted configurations with $d_s \neq 0$ nm (this kind of configuration is widely used to avoid the numerical errors for calculating S parameters at the inhomogeneous interfaces). As we known the surface waves fade out exponentially in the free space, so we use a d_s around λ_0 to diminish the effects of surface waves (λ_0 is the wavelength in free space).

In this paper, d_s = 1550 nm has been taken as an example, and the retrieved parameters have been recalculated and plotted in Figure 3. Compared with the results of d_s = 0 nm, it is obvious that different parameters have been obtained for one unit cell and two unit cells. But when the number of unit cells is larger than three, the retrieved $n_{\rm eff}$ nearly all overlapped those of the infinite periodic nanostructures again. Additionally, similar phenomena have also been found in Figure 3(b) for the other retrieved electromagnetic parameter, i.e., the effective impedance $z_{\rm eff}$. Because of the same retrieved results, the retrieved results of 4 and 5 unit cells have been omitted from Figure 3 for the sake of clarity. From the above results, we can conclude that for this PC near $f_{\rm nor}$ = 0.2858 three-unit-cells thick is the minimum thickness requirement for achieving converged retrieved parameters.

Definitely, the convergency of the retrieved parameters are determined by the resonant interactions between the electromagnetic waves and the periodic structures, which is the

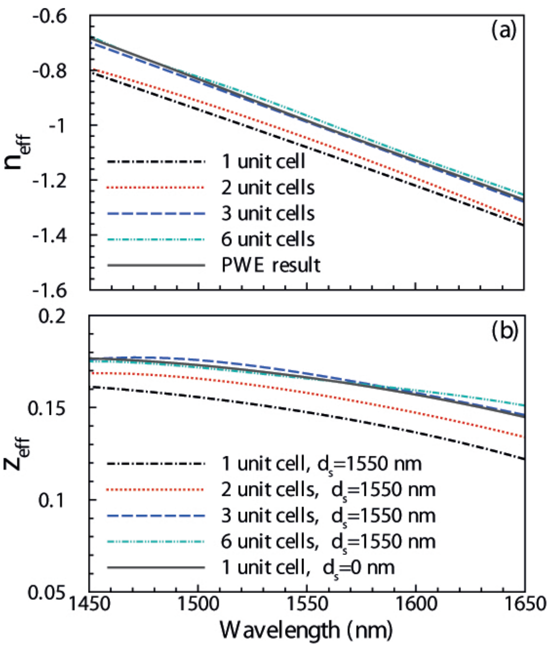

FIG. 3 (a) Retrieved effective refractive index $n_{\rm eff}$ and (b) impedance $z_{\rm eff}$ with d_s = 1550 nm for different number of unit cells. The $n_{\rm eff}$ obtained by utilizing the PWE method and the $z_{\rm eff}$ with d_s = 0 nm for one unit cell are added to (a) and (b), respectively.

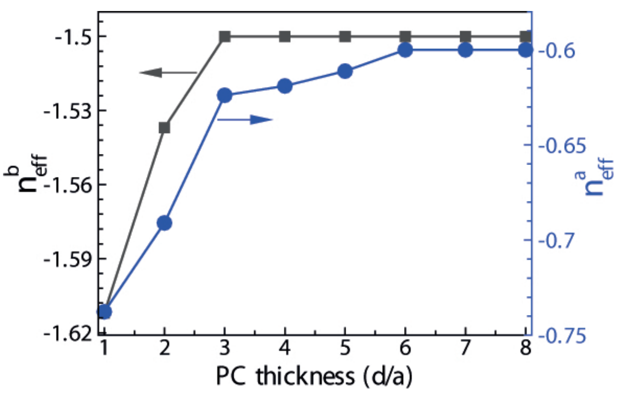

FIG. 4 Retrieved effective refractive index $n_{\rm eff}$ as the function of the PC thickness with d_s = 1550 nm.

physical origin of the abnormal dispersion of PCs, To establish these interactions basically, the periodic nanostructures should be thick enough to hold nearly one whole oscillation. In other words, the nanostructures' thicknesses at least are close to the wavelengthes of the propagating waves in the nanostructure. This suggests a thickness condition under which the retrieved effective electromagnetic parameters can be used to characterize the finite periodic nanostructures.

To verify the above deduction, we analyzed the dependence of the retrieved effective refractive index $n_{\rm eff}$ on the layer thickness with d_s = 1550 nm for another two normalized frequencies, i.e., $f^a_{\rm nor}$ = 0.32 and $f^b_{\rm nor}$ = 0.263. As shown in Figure 4, for $f^a_{\rm nor}$ = 0.32 the retrieved refractive index converges to $n^a_{\rm eff} = -0.6$ when the slab is thicker than $5a$. Moreover, the wavelength in PC slab at this frequency is $\lambda_a = a/f^a_{\rm nor}\left|n^a_{\rm eff}\right| = 5.21a$. For $f^b_{\rm nor} = 0.263$, the minimum thickness for achieving the convergence of $n^b_{\rm eff}$ changes to $3a$ and the wavelength in PC slab is $\lambda_b = a/f^b_{\rm nor}\left|n^b_{\rm eff}\right| = 2.53a$. It is obvious that the retrieved parameters converge when the slab thickness is close to the wavelength of the propagating wave in the PCs.

In addition, similar calculations were performed to check our assumptions in the fishnet metamaterials. We took the same model discussed in the Refs. [22] and [28]. Due to its inhomogeneous interfaces, these two recorders were placed far away from the interfaces of the fishnet metamaterial. The retrieved effective refractive index $n_{\rm eff}$ as a function of the layer numbers were plotted in Figure 5. For the wavelength in vacuum λ_c = 1811 nm, the retrieved $n^c_{\rm eff}$ waves with the layer numbers at first and converges to -2.0 at last when the thickness of the fishnet MMs exceeds $11a_z$, where $a_z = 2t + s$ (t and s correspond to the thickness of metallic cladding (Ag) and dielectric spacer (MgF_2)) is the unit thickness. For this model, a_z = 80 nm and $11a_z$ = 880 nm $\approx \lambda_c/\left|n^c_{\rm eff}\right|$. The same thing takes place for the wavelength in vacuum λ_d = 1763 nm whose retrieved $n^d_{\rm eff}$ are converged to -1.55 until the layer numbers

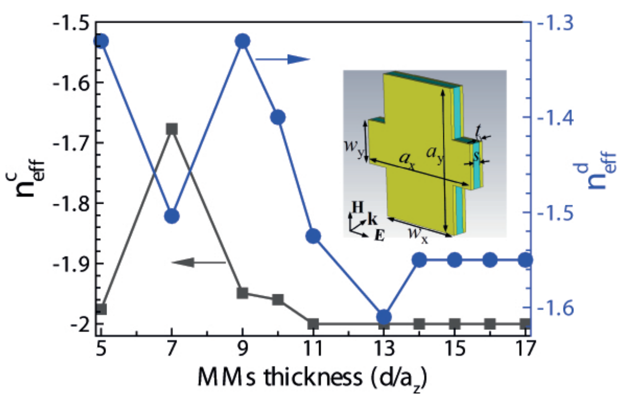

FIG. 5 Retrieved effective refractive index $n_{\rm eff}$ as the function of the fishnet metamaterials (MMs) thickness with d_s = 1811 nm for $n^c_{\rm eff} = -2.0$ and d_s = 1763 nm for $n^d_{\rm eff} = -1.55$. Inset shows the MMs design and polarization configuration. The geometric parameters are $a_x = a_y$ = 860 nm, w_x = 565 nm, w_y = 265 nm. t = 15 nm and s = 50 nm are corresponding to the thickness of metallic cladding (Ag) and dielectric spacer (MgF_2). A Drude model is used for the dielectric parameters of silver, with plasma frequency ω_p = 9.0 eV and scatting frequency γ = 0.054 eV. The dielectric constant of the MgF_2 is ϵ_r = 1.9.

are larger than $\lambda_d / \left| n_{\text{eff}}^d \right| / a_z \approx 14$. We should mention here that, although the lattice constant of the fishnet metamaterial along the light propagation direction is far less than the wavelength, the others are of the same order of magnitude to the wavelength [34]–[36].

4 CONCLUSION

In summary, we have presented a thickness condition under which the periodic nanostructures, such as PCs and metamaterials, can be characterized by the effective electromagnetic parameters within the single-Bloch-mode approximation. This thickness condition, which has been demonstrated in a photonic crystal and in a typical fishnet metamaterial respectively, will be helpful for the design of ultrathin periodic nanostructure-based optical devices.

Although we have only discussed a specific square lattice PC and fishnet metamaterial, this conclusion can be extended to other nanostructures with abnormal dispersion. However, we should point out that the thickness condition is unsuitable for the nanostructures in the traditional long-wavelength limit due to different physical origins.

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