Effective-medium theory for one-dimensional gratings

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(Received 3 December 2014; revised manuscript received 4 May 2015; published 22 May 2015)

Based on a mode-expansion theory under single-mode approximation, we derived the scatterings parameters for a general one-dimensional photonic grating composed of two different materials, and then established an effective-medium theory for such a composite by equating the obtained scattering parameters to those of a homogeneous medium. Our effective-medium theory well describes the grating structures with general material and geometrical parameters, and recovers two previous formulas, which are valid only at certain limiting conditions. The theory is justified by full-wave simulations and microwave experiments.

DOI: 10.1103/PhysRevB.91.174201

PACS number(s): 78.67.Pt, 81.05.Xj, 78.20.Ci, 77.22.Ch

I. INTRODUCTION

Metamaterials are electromagnetic composites constructed by subwavelength-sized microstructures, and thus can exhibit tailored effective permittivity ε and permeability μ . Metamaterials have attracted much attention recently due to their strong abilities to manipulate electromagnetic waves, leading to many fascinating physical effects unattainable in naturally existing materials [1–7]. In this research field, effective-medium theory plays a crucial role since it serves as a bridge to link theories, which are frequently conducted on model hypothetical systems, and experiments, which are always performed on realistic metamaterial systems with complex microstructures. Therefore, a good effective-medium theory, which can precisely predict the effective parameters of complex metamaterials, is always highly desired.

As a particular class of metamaterial, grating structures consisting of alternative stacking of two layers with subwavelength thicknesses and distinct electromagnetic properties [see Fig. 1(a)] have been widely studied in recent years. Many interesting physical effects were discovered based on such structures, such as hyperlensing [8–10], focusing [11], cloaking [12,13], slow-light transport [14], and radiation lift-time engineering [15–18]. To describe the electromagnetic properties of these systems, one frequently used the standard formulas in which the effective ε , or the inverse of effective ε , is written as a volume average of local permittivity or the inverse of local permittivity, depending on the polarization [19,20]. However, since these formulas were derived in the long wavelength limit, they are valid only for grating structures strictly satisfying the long-wavelength-limit condition, that is, the optical thicknesses of both layers should be much smaller than the input wavelength. Whenever the permittivity and/or permeability of a single layer exhibits very large values, such long-wavelength-limit formulas become invalid, even though the whole system still satisfies the subwavelength condition (i.e., the lattice constant of the grating is smaller than wavelength). On the other hand, based on the modeexpansion theory, a delicate approach [21,22] was proposed to homogenize such AB systems, which does not require a strict long-wavelength-limit condition. Unfortunately, the developed theory is limited to the special case that one layer must be a perfect electric conductor (PEC) [21]. Given so many interesting applications/phenomena already discovered based on these systems [8–18], and given considerable efforts made on developing appropriate effective-medium descriptions for such systems [23–28], we feel that an effective-medium theory for such grating structures, which is valid under more general conditions, is highly desired.

In this work, we establish a theory to study the effectivemedium properties of one-dimensional gratings with arbitrary constitutional and geometrical parameters. Our effectivemedium theory not only recovers those previously derived formulas valid only at certain limiting conditions, but works well far beyond these limitations to nearly cover the whole parameter spaces as long as the subwavelength condition is satisfied. Finite-difference-time-domain (FDTD) simulations and microwave experiments are performed on realistic structures to justify our theory.

Our paper is organized as follows. We first derive the effective-medium theory in Sec. II, and then justify its validity in Sec. III by full-wave simulations. Section IV is devoted to a detailed comparison between our effective-medium theory and two previous formulas. After presenting the experimental confirmation of our effective-medium theory in Sec. V, we conclude the paper in Sec. VI.

II. EFFECTIVE-MEDIUM THEORY

Figure 1 schematically depicts the geometry of our system, whose unit cell contains two layers with thicknesses d_A and d_B , and electromagnetic parameters ε_A, μ_A and ε_B, μ_B . We are primarily interested in the effective permittivity $\varepsilon_{\text{eff}}^{xx}$ of the structure, since it is this component that caused strong debates and confusions in previous studies [24–26]. To study $\varepsilon_{\text{eff}}^{xx}$, we assume that a transverse-magnetic (TM) polarized light (with $\vec{E}||\hat{x})$ is normally coupled into the grating through the xy

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FIG. 1. (Color online) Schematic picture of (a) the grating structure under study and (b) its effective medium model.

interface [Fig. 1(a)], and study the corresponding light scattering problem. Obviously, light scatterings at this interface cannot be studied by a simple 2 × 2 transfer-matrix method (TMM), since higher-order diffractions are inevitable [see Fig. 1(a)]. Our strategy to determine the effective parameters $\varepsilon_{\text{eff}}^{xx}, \mu_{\text{eff}}^{yy}$ of the given system is described as follows. We first employ the rigorous mode-expansion theory to calculate the scattering coefficients of the system [Fig. 1(a)], and then derive analytical formulas for the zero-order transmission/reflection coefficients based on a single-mode approximation. Finally, the effective-medium parameters are fixed by equating the obtained zero-order scattering coefficients to those of a homogeneous medium under the same illuminations [Fig. 1(b)]. Without causing confusion, in what follows we neglect the superscripts xx and yy in $\varepsilon_{\text{eff}}^{xx}$ and μ_{eff}^{yy} .

According to the mode-expansion theory, we need to first expand the electromagnetic fields to linear combinations of eigenmodes in different regions. For the present configuration, electromagnetic eigenmodes in region I (air region above the grating, see Fig. 1) are just diffraction modes, which are TMpolarized plane waves taking parallel wave vectors $k_{x,n}^{(I)} = n \cdot$ $2\pi/d$ $(n = 0, \pm 1, \pm 2, ...)$ with $d = d_A + d_B$ being the periodicity of our system. The corresponding field patterns are denoted by $[\vec{E}_n^{(I)}(x), \vec{H}_n^{(I)}(x)]e^{\pm ik_{z,n}^{(I)} \cdot z}$ where $k_{z,n}^{(I)} = \sqrt{k_0^2 - (k_{x,n}^{(I)})^2}$ with $k_0 = \omega/c$ and \pm denote forward and backward modes, respectively. In region II, which is the semi-infinite space occupied by the grating, the relevant electromagnetic eigenmodes are a series of Bloch waves characterized by Bloch wave vectors $K_{x,q} = q \cdot 2\pi/d$ with $q = 0, \pm 1, \pm 2, \ldots$ Since region II exhibits translation-invariant symmetry along the zaxis, the eigen-wave-functions in this region can be written in general as $[\vec{E}_q^{(\text{II})}(x), \vec{H}_q^{(\text{II})}(x)]e^{\pm ik_{z,q}^{(\text{II})} \cdot z}$ with perpendicular wave vectors $k_{z,q}^{(II)}$ being unknown parameters to be determined. Meanwhile, eigenmodes in such AB periodic systems can be studied by a standard TMM imposing the Bloch condition along the x direction, i.e., $\vec{E}_q^{(\text{II})}(x+d) = e^{iK_{x,q}d}\vec{E}_q^{(\text{II})}(x)$ and $\vec{H}_q^{(\text{II})}(x+d) = e^{iK_{x,q}d}\vec{H}_q^{(\text{II})}(x)$. A straightforward calculation shows that, given a frequency ω and thus $k_0 = \omega/c$, $k_{z,q}^{(\text{II})}$ are correlated with the Bloch wave vector $K_{x,q}$ by the following equation [29] (see Appendix A),

$$2\cos\left(k_{x}^{A}d_{A}+k_{x}^{B}d_{B}\right)-\left(\frac{\varepsilon_{B}k_{x}^{A}}{\varepsilon_{A}k_{x}^{B}}+\frac{\varepsilon_{A}k_{x}^{B}}{\varepsilon_{B}k_{x}^{A}}-2\right)$$
$$\times\sin\left(k_{x}^{A}d_{A}\right)\sin\left(k_{x}^{B}d_{B}\right)=2\cos(K_{x,q}d),\qquad(1)$$

where

$$k_{x}^{A} = \sqrt{\varepsilon_{A}\mu_{A}k_{0}^{2} - (k_{z,q}^{(\text{II})})^{2}}, \quad k_{x}^{B} = \sqrt{\varepsilon_{B}\mu_{B}k_{0}^{2} - (k_{z,q}^{(\text{II})})^{2}}.$$
 (2)

Solving Eq. (1) yields a series of $k_{z,q}^{(\text{II})}$ for all eigenmodes. The corresponding wave functions $[\vec{E}_q^{(\text{II})}(x), \vec{H}_q^{(\text{II})}(x)]$ can be easily obtained by the TMM calculations.

With eigenmodes in both regions known, we can formally express the total *E* fields in different regions as

$$\vec{E}_{\text{total}}^{(\text{I})}(x,z) = \vec{E}^{\text{inc}}(x)e^{ik_0\cdot z} + \sum_n r_n \vec{E}_n^{(\text{I})}(x)e^{-ik_{z,n}^{(\text{I})}\cdot z}$$

$$\vec{E}_{\text{total}}^{(\text{II})}(x,z) = \sum_q t_q \vec{E}_q^{(\text{II})}(x)e^{ik_{z,q}^{(\text{II})}\cdot z},$$
(3)

where $\vec{E}^{inc}(x)e^{ik_0\cdot z} = \vec{E}_0^{(I)}(x)e^{ik_0\cdot z}$ is the incident field, r_n denotes the reflection coefficient for the *n*th mode in region I and t_q the transmission coefficient for the *q*th mode in region II. *H* fields satisfy two similar equations. We note that **E** and **H** components of these eigenmodes are not totally independent, but rather correlated with each other via

$$E_{n,x}^{(I)}(x) = \frac{k_{z,n}^{(I)}}{\omega \varepsilon_0} H_{n,y}^{(I)}(x)$$

$$E_{q,x}^{(II)}(x) = \frac{k_{z,q}^{(II)}}{\omega \varepsilon_0 \varepsilon(x)} H_{q,y}^{(II)}(x),$$
(4)

where we have defined $\varepsilon(x) = \varepsilon_A$ for x located inside layer A and $\varepsilon(x) = \varepsilon_B$ for x located inside layer B. According to the field continuity conditions at the z = 0 interface, we get from Eq. (3) that

$$E_{0,x}^{(I)}(x) + \sum_{n} r_{n} E_{n,x}^{(I)}(x) = \sum_{q} t_{q} E_{q,x}^{(II)}(x)$$

$$H_{0,y}^{(I)}(x) + \sum_{n} r_{n} H_{n,y}^{(I)}(x) = \sum_{q} t_{q} H_{q,y}^{(II)}(x).$$
(5)

We can use the orthonormal properties of those eigenmodes to derive the equations satisfied by the expansion parameters $\{r_n, t_q\}$. In region I, it is easy to verify that eigenmodes (diffraction modes) satisfy the following orthonormal conditions

$$\int_{u.c.} \left[E_{m,x}^{(I)}(x) \right]^* \cdot E_{n,x}^{(I)}(x) dx = \delta_{m,n}, \tag{6}$$

where the integrals are performed within a unit cell. The orthonormal conditions for $H_{n,y}^{(I)}(x)$ can be derived from Eqs. (4) and (6). However, things are quite nontrivial for the eigenmodes inside region II, where the orthonormal conditions should now be written as

$$\int_{u.c.} \left(\frac{1}{\varepsilon(x)} H_{q,y}^{(\mathrm{II})}(x)^* \cdot H_{q',y}^{(\mathrm{II})}(x) \right) dx = \delta_{qq'}, \tag{7}$$

in which a metric term $1/\varepsilon(x)$ must be added [30] (see Appendix B). Again, the orthonormal conditions for $E_{q,x}^{(II)}(x)$ can be derived from Eqs. (7) and (4) [30]. In the limiting case of one layer being PEC (i.e., let $\varepsilon_A(x) \to -\infty$), we note that both **E** and **H** fields vanish inside layer A so that Eq. (7) recovers the conventional orthonormal conditions satisfied by the waveguide modes in layer B sandwiched by two PEC walls (e.g., Eq. (A7) in Ref. [31]). Employing the two orthonormal conditions Eqs. (6)–(7) [32], we can derive from Eq. (5) a set of equations to determine the expansion coefficients,

$$(1 - r_0) (S_{0q}^{\rm H})^* + \sum_{n \neq 0} \left[r_n (S_{nq}^{\rm H})^* \right] = t_q$$

$$\delta_{n0} + r_n = \sum_q t_q S_{nq}^{\rm E}, \qquad (8)$$

where the S parameters are defined by

$$S_{nq}^{\rm E} = \int_{u.c.} \left(E_{n,x}^{({\rm I})} \right)^* \cdot E_{q,x}^{({\rm II})} dx$$

$$S_{nq}^{\rm H} = \int_{u.c.} \left(H_{n,y}^{({\rm I})} \right)^* \cdot \frac{1}{\varepsilon(x)} H_{q,y}^{({\rm II})} dx,$$
(9)

which represent the overlapping between different modes in two regions.

In principle, the scattering coefficients $\{t_q, r_n\}$ can be obtained by numerically solving Eq. (8) with enough modes considered. To retrieve the effective-medium properties of the system, we need to derive the analytical formulas for the zero-order scattering coefficients, which can be done based on a single-mode approximation [i.e., retaining only the fundamental modes (labeled by indexes n = 0, q = 0) in both regions]. Such an approximation is justified when the effective overlapping integral between two fundamental modes $(S_{00})^2 = S_{00}^{\rm E} \cdot (S_{00}^{\rm H})^*$ is the dominant term among all overlapping integrals $(S_{nq})^2 = S_{nq}^{\rm E} \cdot (S_{nq}^{\rm H})^*$. Under such an approximation, we can solve Eq. (8) rigorously to get the reflection coefficient for the specular mode as

$$r_0 = \frac{(S_{00})^2 - 1}{(S_{00})^2 + 1}.$$
(10)

Mapping our system to a homogeneous medium [see Fig. 1(b)] with effective parameters $\varepsilon_{\text{eff}}, \mu_{\text{eff}}$, and noting that the reflection coefficient at the surface of such a medium is $r_0 = (Z_{\text{eff}} - 1)/(Z_{\text{eff}} + 1)$ with $Z_{\text{eff}} = \sqrt{\mu_{\text{eff}}}/\sqrt{\varepsilon_{\text{eff}}}$, we found that the effective impedance of our grating structure is

$$Z_{\rm eff} = (S_{00})^2. \tag{11}$$

On the other hand, since we only consider the fundamental mode inside the grating, which is characterized by a wave vector $k_{z,0}^{(II)}$, mapping our medium to a homogeneous effective medium means that the effective refraction index of the grating must be

$$n_{\rm eff} = \sqrt{\varepsilon_{\rm eff}} \cdot \sqrt{\mu_{\rm eff}} = k_{z,0}^{\rm (II)} / k_0. \tag{12}$$

Solving Eqs. (11)–(12), we finally get the following analytical formulas

$$\varepsilon_{\rm eff} = \frac{k_{z,0}^{\rm (II)}}{k_0 \cdot (S_{00})^2}$$

$$\mu_{\rm eff} = \frac{k_{z,0}^{\rm (II)} \cdot (S_{00})^2}{k_0}$$
(13)

to determine the effective parameters of our grating medium. Two involved physical quantities, $k_{z,0}^{(II)}$, $(S_{00})^2$, can be computed by solving Eqs. (1)–(2) and (9).

At this point, it is helpful to discuss under what conditions the single-mode approximation is valid. In most cases where the subwavelength condition $d \ll \lambda$ is satisfied, such an approximation is valid since all high-order diffraction modes in air are evanescent waves and the high-order modes inside the grating take imaginary wave vectors due to the subwavelength confinement in lateral directions. However, we will show that in some particular situations, such an approximation becomes invalid even though the subwavelength condition is still satisfied.

III. VALIDATIONS BY NUMERICAL SIMULATIONS

We employ full-wave simulations to verify the newly established effective-medium theory based on two representative examples. The first example is a dielectric/air grating with parameters $\varepsilon_A = 40, \mu_A = 1, \varepsilon_B = \mu_B = 1$, and $d_A = 3d_B$. For any frequency satisfying the subwavelength condition, i.e., $k_0 d/2\pi \ll 1$, we can employ our theory to determine the effective parameters of the structure. $\varepsilon_{\rm eff}$ and $\mu_{\rm eff}$ thus obtained are plotted in Fig. 2(a) as functions of frequency. In the long wavelength limit where $k_0 d/2\pi \rightarrow 0$, we find that the calculated $\varepsilon_{\rm eff}$ and $\mu_{\rm eff}$ approach to those values obtained by standard volume average method [20], i.e., $\bar{\varepsilon} = 3.721$ and $\bar{\mu} = 1$. However, deviations from these long-wavelengthlimit values become non-negligible as frequency increases, especially for μ_{eff} . These results appear quite counterintuitive at first glance since the constitutional materials constructing our grating are all purely dielectric. Such a magnetic response, although very weak here, must be contributed by displacement currents excited inside the dielectric layers.



FIG. 2. (Color online) (a) Effective parameters of a dielectric/air grating calculated by our effective-medium theory. (b) Transmission and reflection spectra of a 15*d*-thick slab of such grating structure, calculated by FDTD simulations on realistic system (symbols) and our effective-medium theory on model system (lines). Here the constitutional parameters are $\varepsilon_A = 40, \mu_A = 1, \varepsilon_B = \mu_B = 1$, and $d_A = 3d_B$.



FIG. 3. (Color online) Transmittance and reflectance for two slabs of AB gratings with different thicknesses *h*, calculated by FDTD simulations on realistic systems (symbols) and our effective-medium theory on model systems (lines). Here, the working wavelength is fixed as $\lambda = 25d$. In these AB structures, the B layer is always fixed as air while the A layer is a dielectric with (a) $\varepsilon_A = 40$ and a metal with (b) $\varepsilon_A = -100$.

To justify our effective-medium theory, we employ FDTD simulations to calculate the transmission/reflection spectra of electromagnetic waves through a slab of such AB grating with thickness h = 15d, and then compare in Fig. 2(b) the FDTD results with those calculated by a standard TMM on a homogeneous slab of the same thickness with electromagnetic parameters given by ε_{eff} , μ_{eff} as shown in Fig. 2(a). Excellent agreement is noted between FDTD and the effective-medium-theory results in the whole frequency region considered. We next fix the wavelength at $\lambda = 25d$ to compute the transmittance and reflectance of electromagnetic waves through a series of slabs of our gratings with different thicknesses *h*. Comparison between FDTD and effective-medium theory shown in Fig. 3(a) indicates that our theory can well reproduce the full-wave simulations on realistic structures.

The second example we study is a metal/air grating, which was frequently studied in the literature as a hyperbolic metamaterial [21,27,33]. The unit cell is the same as that of the first example, only with the A layer replaced by a metal layer described by a Drude-like dielectric function $\varepsilon_A = 1 - \lambda^2 / \lambda_p^2$ with $\lambda_p = 1.875d$ denoting the plasmon wavelength. We employ our effective-medium theory to calculate $\varepsilon_{\rm eff}, \mu_{\rm eff}$ of this system and plot the obtained results in Fig. 4(a). Compared with the case of dielectric AB grating [see Fig. 2(a)], we find the present metal/air grating exhibits a diamagnetic response with $\mu_{\rm eff}$ < 1. We also note that even at very low frequencies, the calculated $\mu_{\rm eff}$ does not converge to the longwavelength-limit value $\bar{\mu} = 1$, indicating the failure of the naïve long-wavelength-limit formulas in studying this system. Such a strong diamagnetic response has been noted in previous studies [34]. Again, to justify our effective-medium theory, we perform two series of FDTD simulations similar to those for the dielectric/air systems, and compare the results with



FIG. 4. (Color online) (a) Effective parameters of a metal/air grating calculated by the effective-medium theory. (b) Transmission and reflection spectra of a 15*d*-thick slab of such grating structure, calculated by FDTD simulations on realistic system (symbols) and the effective-medium theory on model system (lines). Here the constitutional parameters are $\varepsilon_A = 1 - \lambda^2/\lambda_p^2$ with $\lambda_p = 1.875d$, $\mu_A = 1$, $\varepsilon_B = \mu_B = 1$, and $d_A = 3d_B$.

those calculated by our effective-medium theory. Comparisons shown in Fig. 3(b) and Fig. 4(b) justified our effective-medium theory for such a system.

IV. COMPARISONS WITH PREVIOUS THEORIES

Our effective-medium theory can cover two previously developed formulas under certain limiting conditions. Consider first the limit of $\varepsilon_A \rightarrow -\infty$ when layer A becomes a PEC so that both the **E** and **H** field inside layer A are exactly 0. In such a case, the fundamental mode in the AB structure is just a transverse electromagnetic waveguide mode trapped only inside layer B with wave vector given by $k_{z,0}^{(II)} = k_0 \sqrt{\varepsilon_B \mu_B}$. Meanwhile, it is straightforward to use the normalized wave function of such a transverse electromagnetic mode to demonstrate that $S_{00}^{\rm E} = \frac{k_0}{\omega \varepsilon_0} \sqrt{\frac{\mu_B d_B}{d}}$, $S_{00}^{\rm H} = \frac{\omega \varepsilon_0}{k_0} \sqrt{\frac{d_B}{\varepsilon_B d}}$, and thus

$$(S_{00})^2 = \sqrt{\frac{\mu_B}{\varepsilon_B}} \frac{d_B}{d}.$$
 (14)

Putting the above results into Eq. (13), we find the effective parameters are now given by

$$\varepsilon_{\rm eff} = \varepsilon_B d/d_B$$

$$\mu_{\rm eff} = \mu_B d_B/d,$$
(15)

which are just the results obtained by the PEC-based effectivemedium theory for such systems [21].

Consider the second limiting case that $\lambda_0/\sqrt{\varepsilon_A \mu_A} \gg d_A$, $\lambda_0/\sqrt{\varepsilon_B \mu_B} \gg d_B$, which represents the true long wavelength limit. In this limit, noting that $k_{z,0}^{(\text{II})}$ is of the same order with k_0 ,

we thus expect that both $k_x^A d_A$ and $k_x^B d_B$ are small parameters [see Eq. (2)]. Expanding Eq. (1) in terms of $k_x^A d_A$ and $k_x^B d_B$, and only retaining the leading-order terms, we get

$$\left(k_x^A d_A\right)^2 + \left(k_x^B d_B\right)^2 + \left(\frac{\varepsilon_B k_x^A}{\varepsilon_A k_x^B} + \frac{\varepsilon_A k_x^B}{\varepsilon_B k_x^A}\right) \left(k_x^A d_A\right) \left(k_x^B d_B\right) = 0.$$
(16)

Putting Eq. (2) into Eq. (16), we solve the resultant equation to get

$$\left(k_{z,0}^{(\text{II})}\right)^{2} = \frac{\mu_{A}d_{A} + \mu_{B}d_{B}}{\varepsilon_{A}^{-1}d_{A} + \varepsilon_{B}^{-1}d_{B}}k_{0}^{2}.$$
(17)

Let us now check the overlapping functions $S_{00}^{\rm E}$ and $S_{00}^{\rm H}$. Since $k_x^A d_A \rightarrow 0$ and $k_x^B d_B \rightarrow 0$, we expect that H_y does not vary too much within both layer A and layer B. In addition, considering that H_y should be continuous across the AB boundary, it is a good zero-order approximation to assume that H_y keeps at a constant value within the entire unit cell. Adopting the orthonormal condition Eq. (7), we find that the wave function of the fundamental mode inside region II can be approximately written as

$$H_{0,y}^{({\rm II})} \approx \frac{1}{\sqrt{\varepsilon_A^{-1} d_A + \varepsilon_B^{-1} d_B}}.$$
 (18)

The corresponding wave function for $E_{0,x}^{(\text{II})}$ can be obtained with Eqs. (18) and (4). Put the above results into Eq. (9), we find from simple computations that the two overlapping integrals are

$$S_{00}^{\rm E} = \frac{k_{z,0}^{\rm (II)}}{\omega\varepsilon_0} \sqrt{\frac{\varepsilon_A^{-1}d_A + \varepsilon_B^{-1}d_B}{d}}$$

$$S_{00}^{\rm H} = \frac{\omega\varepsilon_0}{k_0} \sqrt{\frac{\varepsilon_A^{-1}d_A + \varepsilon_B^{-1}d_B}{d}}.$$
(19)

Therefore, the two effective parameters can be derived from Eqs. (19) and (13), which are

$$\varepsilon_{\rm eff} = \frac{d}{\varepsilon_{\rm A}^{-1} d_{\rm A} + \varepsilon_{\rm B}^{-1} d_{\rm B}},$$

$$\mu_{\rm eff} = \frac{\mu_{\rm A} d_{\rm A} + \mu_{\rm B} d_{\rm B}}{d}.$$
(20)

Equation (20) recovers the well-known formulas derived in the long wavelength limit for this polarization [19].

We now compare our effective-medium theory with these two previous formulas under more general conditions. In particular, we will check the validity regions of these different versions of effective-medium theory. To quantitatively describe how good an effective-medium theory is, we define a physical quantity

$$\delta T = \langle |t_{\rm EMT} - t_{\rm FDTD}| \rangle, \qquad (21)$$

which measures the difference between the (complex) transmission coefficient t_{EMT} calculated by a particular effective-medium theory on a homogeneous model system and the FDTD-calculated complex value t_{FDTD} on a realistic inhomogeneous AB grating system. To suppress the accidental fluctuations caused by Fabry-Perot resonances



FIG. 5. (Color online) (a) δT for a series of AB gratings with varying ε_A , calculated by the present effective-medium theory (circles), the PEC-based formula Eq. (15) (triangles), and the long-wavelength-limit formula Eq. (20) (squares). (b) Effective parameters of the systems calculated by the present effective-medium theory, with inset depicting how the two overlapping integrals vary against ε_A .

through a finite-thickness slab, we average $|t_{\rm EMT} - t_{\rm FDTD}|$ over samples with thicknesses varying from 0.25d-15d. The effective-medium theory can be our theory developed here, and can also be the two previous formulas [i.e, Eq. (15) and Eq. (20)]. By computing δT for different versions of effective-medium theory, we can quantitatively check how good these effective-medium theories are in describing the inhomogeneous medium under study.

We now compare these theories by studying a series of AB gratings with B layer fixed as air and with ε_A varying from $-\infty$ to ∞ . Fix the working wavelength as $\lambda = 25d$, we employ different versions of effective-medium theory to compute their corresponding δT 's and compare the results in Fig. 5(a) as functions of ε_A . The effective parameters calculated by the present theory are plotted in Fig. 5(b) for the sake of easy comparison. Figure 5(a) shows clearly that, while the PEC-based formulas [i.e., Eq. (15)] can only work in the limiting case with $\varepsilon_A \rightarrow -\infty$ and the long-wavelength-limit formulas [i.e., Eq. (20)] can only work in two small regions $-40 < \varepsilon_A < -15$ and $0 < \varepsilon_A < 20$, our effective-medium theory works very well in nearly the entire parameter space studied, including those regions where previous formulas do not work at all.

However, in a small shaded region centered at $\varepsilon_A = -3$, all three effective-medium theories do not work well, as shown by the large values of δT calculated by different theories. A simple explanation of such failure is that the effective ε_{eff} is so large near the point of $\varepsilon_A = -3$ that the effective wavelength inside the medium, defined as $\lambda_{\text{eff}} = \lambda_0 / \sqrt{\varepsilon_{\text{eff}} \cdot \mu_{\text{eff}}}$, is significantly enhanced resulting in the failure of the single-mode approximation. Such a simple picture is reinforced by quantitatively calculating the overlapping integrals involving higher-order modes. The inset to Fig. 5(b) depicts how the two most important overlapping integrals, namely $(S_{00})^2$ and $(S_{01})^2$, vary against ε_A . Clearly, the coupling between the first high-order mode inside the grating and the fundamental mode in air becomes significantly enhanced in the shaded region, and it can even compete with the coupling between two fundamental modes in the vicinity of $\varepsilon_A \rightarrow -3$. In fact, the fundamental mode in region II, which is defined as the mode that has the largest overlapping integral with the fundamental mode in region I, changes its wave-function characteristics at the point $\varepsilon_A \rightarrow -3$. Therefore, in such a parameter region, the inner properties inside the grating are no longer solely dominated by a single fundamental mode, so that it is impossible to find an effective-medium theory to homogenize the complex structure. We note that a similar conclusion has also been drawn from a different theoretical approach [24,26]. However, in all other parameter regions as long as the AB grating can be homogenized as an effective medium, our effective-medium theory is always the best one to describe the complex system.

Although here we did not consider the nonlocal responses in developing our effective-medium theory, we note that the theory can be easily extended to include such effects by simply considering the oblique-incidence situations. In fact, we find that our theory, even without considering the nonlocal effects, can still well describe the optical responses of the gratings under oblique incidences (see Appendix C). In addition, we note that the homogenization approach described in this paper is so general that it can also be employed to develop effective-medium theories for more complex structures with two-dimensional microstructures.

V. EXPERIMENTAL VERIFICATIONS

We now perform microwave experiments to verify the newly developed effective-medium theory for onedimensional gratings. To highlight the importance of our effective-medium theory, we purposely choose a parameter region where the previous two formulas do not work well. Figure 5(a) shows that the region where ε_A takes a moderately large negative value is a desired region. However, metal does not exhibit a negative ε in the GHz regime, but rather behaves like a PEC. To realize a negative- ε_A slab, we design and fabricate a three-dimensional metallic mesh structure with subwavelength square openings. Figure 6 (a) shows the picture of the fabricated mesh structure, with the inset depicting a computer-generated zoom-in view of the structure. In the wavelength regime where $\lambda \gg a$ with a being the lattice constant of the mesh, our system is an excellent metamaterial to mimic a negative- ε_A slab, as desired.

By computing the transmission/reflection spectra for a slab of the designed mesh structure, we successfully retrieved the effective permittivity and permeability of the mesh metamaterial by the standard *S*-parameter retrieval method [35]. The simulated results are plotted in Fig. 6(b), where indeed we find that $\varepsilon_{\text{mesh}}$ takes a desired negative value in the frequency region of interest. It is worth noting that μ_{mesh} is significantly smaller than 1, due to the non-negligible diamagnetic effects in such three-dimensional mesh structures.

Having obtained an appropriate material to represent layer A, we next take air as layer B to form an AB grating, and then perform microwave experiments to measure the transmission/reflection spectra of the AB grating. The widths of layer A and layer B are $d_A = 3 \text{ mm}, d_B = 2 \text{ mm}$, respectively, and the total thickness of the constructed AB grating is h = 60 mm. The lateral dimension of the fabricated AB structure is (400 mm × 400 mm, see Appendix D for sample picture).



FIG. 6. (Color online) (a) Picture of the fabricated metallic mesh, with inset depicting a computer-generated zoom-in view of the structure. (b) Effective-medium parameters of the mesh sample, retrieved from FDTD simulations. (c) Effective-medium parameters of the air/mesh grating calculated by our effective-medium theory with $d_{\text{mesh}} = 3 \text{ mm}$ and $d_{\text{air}} = 2 \text{ mm}$. (d) Transmission spectra of the air/mesh grating with thickness h = 60 mm, obtained by measurements (star), FDTD simulations on realistic structures (black lines), and model calculations based on our effective-medium theory (red line) and the long-wavelength-limit formulas (blue line).

Open stars in Fig. 6(d) are the measured transmittance spectrum of the fabricated sample, which is in good agreement with FDTD simulations on realistic structures. In our experiments, we have adopted the time-domain gating technique to avoid multiple reflections between the source and receiver horns (see Appendix D for experimental details). Meanwhile, knowing the electromagnetic and geometric properties of the constructional A and B layers, we employ our effective-medium theory



FIG. 7. (Color online) Reflectance for two slabs of AB gratings under different incident angles, calculated by FDTD simulations on realistic systems (symbols) and our effective-medium theory on model systems (lines). Here, the working wavelength is fixed as $\lambda = 25d$. In these AB structures, the B layer is always fixed as air while the A layer is a dielectric with (a) $\varepsilon_A = 40$ and a metal with (b) $\varepsilon_A = -100$.

to compute the effective parameters of the resultant AB grating structure, and depict the results in Fig. 6(c). Using these effective parameters, we employ the standard TMM to calculate the transmission spectra through a model homogeneous slab with thickness h = 60 mm. Figure 6(d) shows that our effective-medium theory can well reproduce both measured and FDTD simulated transmittance spectra. In contrast, if we derive the effective parameters based on the long-wavelengthlimit formulas [i.e., Eq. (20)], we find that the corresponding transmission spectra calculated by such a model show significant deviations from the experimental results. Results calculated by PEC-based effective-medium theory [i.e., Eq. (15)] show even stronger deviations from the experimental and FDTD results and are not included in Fig. 6(d). Such a comparison unambiguously validates the newly established effectivemedium theory and highlights the importance of adopting our theory to describe such a grating in general cases, especially in those cases where previous theories do not work well.

VI. CONCLUSIONS

In summary, we established an effective-medium theory to homogenize a grating structure consisting of two different layers with distinct electromagnetic properties. Our theory can recover two previously developed formulas, which are valid only at certain limiting conditions, and more importantly, still works well in parameter spaces where previous formulas fail. We performed microwave experiments and full-wave simulations to successfully validate our theory.

ACKNOWLEDGMENTS

This work was supported by the National Natural Science Foundation China (Grants No. 11474057, No. 11174055, No. 11204040, No. 51322201, and No. 11404063), and Shanghai Science and Technology Committee (Grant No. 14PJ1401200).

APPENDIX A: DERIVATION OF EQ. (1)

Consider the propagation of a transverse-magnetic (TM) mode (with nonzero field components E_x, E_z, H_y) in such an AB structure [see Fig. 1(a)]. Matching boundary conditions and using the transfer-matrix method (TMM) [29], we find that the evolution of $H_y(x)$ field across a unit cell in an AB structure can be written as

$$\begin{pmatrix} H_{\rm B}^+(d) \\ H_{\rm B}^-(d) \end{pmatrix} = T_{\rm B} M_{\rm BA} T_{\rm A} M_{\rm AB} \begin{pmatrix} H_{\rm B}^+(0) \\ H_{\rm B}^-(0) \end{pmatrix}$$
$$= \mathcal{Q} \begin{pmatrix} H_{\rm B}^+(0) \\ H_{\rm B}^-(0) \end{pmatrix},$$
(A1)

where

$$T_{A} = \begin{pmatrix} e^{iP_{A}} & 0\\ 0 & e^{-iP_{A}} \end{pmatrix}, \quad T_{B} = \begin{pmatrix} e^{iP_{B}} & 0\\ 0 & e^{-iP_{B}} \end{pmatrix}, \quad (A2)$$
$$M_{BA} = \frac{1}{2} \begin{pmatrix} (1+\Delta) & (1-\Delta)\\ (1-\Delta) & (1+\Delta) \end{pmatrix}, \\M_{AB} = \frac{1}{2} \begin{pmatrix} (1+\Delta^{-1}) & (1-\Delta^{-1})\\ (1-\Delta^{-1}) & (1+\Delta^{-1}) \end{pmatrix}$$
(A3)

in which $P_A = k_x^A d_A$, $P_B = k_x^B d_B$, $\Delta = \frac{\varepsilon_B k_x^A}{\varepsilon_A k_x^B}$, and $d = d_A + d_B$ is the length of a unit cell. Here + and – denote the field components for waves propagating to +x and -x directions. Imposing the Bloch condition, we find that eigenmodes (with TM polarization) in region II must satisfy

$$Tr[Q] = 2\cos Kd \tag{A4}$$

with *K* being the Bloch wave-vector. Putting Eqs. (A1)–(A3) into (A4), we get an equation that is just Eq. (1) in the main text.

APPENDIX B: DERIVATION OF EQ. (7)

As discussed in Ref. [30], the most general form of a second-order linear differential operator is

$$\hat{\mathcal{L}} = p(x)\frac{d^2}{dx^2} + p_0(x)\frac{d}{dx} + q(x).$$
 (B1)

If $p(x), p_0(x), q(x)$ are all real functions and the condition

$$\frac{d}{dx}p(x) = p_0(x) \tag{B2}$$

is satisfied, $\hat{\mathcal{L}}$ is called a self-adjoint operator and can be rewritten as

$$\hat{\mathcal{L}} = \frac{d}{dx} \left[p(x) \frac{d}{dx} \right] + q(x).$$
(B3)

The most remarkable property of a self-adjoint operator is that it satisfies

$$\langle v | \hat{\mathcal{L}} u \rangle = \langle \hat{\mathcal{L}} v | u \rangle, \tag{B4}$$

where u(x), v(x) are two arbitrary complex functions defined in a bounded region [a,b], and $\langle v | \hat{\mathcal{L}} u \rangle = \int_a^b v^*(x) \cdot \hat{\mathcal{L}} u(x) dx$, $\langle \hat{\mathcal{L}} v | u \rangle = \int_a^b (\hat{\mathcal{L}} v(x))^* \cdot u(x) dx$ define the inner products between two relevant functions. Note that either periodic or vanishing boundary condition should be specified at the domain boundary in deriving Eq. (B4).

In general, a self-adjoint operator can have the following eigenfunction equation

$$\hat{\mathcal{L}}u(x) - \lambda w(x)u(x) = 0, \tag{B5}$$

where λ and u(x) are the eigenvalue and associated eigenfunction, respectively, and w(x) is a real function called the weight function (metric factor). For any two different eigenvalues λ_i, λ_j and their associated eigenfunctions $u_i(x), u_j(x)$, according to Eq. (B4), we must have

$$\hat{\mathcal{L}}u_i(x) = \lambda_i w(x)u_i(x), \quad \hat{\mathcal{L}}u_j(x) = \lambda_j w(x)u_j(x).$$
(B6)

Meanwhile, the self-adjoint property Eq. (B4) ensures that

$$\langle u_i | \hat{\mathcal{L}} u_i \rangle = \langle \hat{\mathcal{L}} u_i | u_i \rangle. \tag{B7}$$

Therefore, putting Eq. (B5) into Eq. (B7), we get

$$(\lambda_i - \lambda_j) \langle u_i | w u_j \rangle = 0.$$
 (B8)

Since $\lambda_i - \lambda_j \neq 0$, we have the following generalized orthogonal condition for any two different modes,

$$\langle u_i | w u_j \rangle = \delta_{ij}. \tag{B9}$$



FIG. 8. (Color online) (a) Picture of the AB grating; (b) schematics of the experimental setup.

We now use the above general knowledge to study our problem. In our case, we consider a TM mode propagating inside the AB structure described by relative permittivity $\varepsilon(x)$ and permeability $\mu(x)$. Based on Maxwell's equations, we obtain the wave equation satisfied by the H_y component, which can be rewritten as the following form

$$\frac{\partial}{\partial x} \left(\frac{\partial H_y(x)}{\varepsilon(x)\partial x} \right) + \left(k_0^2 \mu(x) - \frac{k_z^2}{\varepsilon(x)} \right) H_y(x) = 0, \quad (B10)$$

with $k_0^2 = \omega^2/c^2$. Comparing Eq. (B10) with Eqs. (B5) and (B3), we find that k_z^2 and $H_y(x)$ are the eigenvalue and eigenwave-function of a self-adjoint operator $\hat{\mathcal{L}} = \frac{d}{dx} \left[\frac{1}{\varepsilon(x)} \frac{d}{dx} \right] + k_0^2 \mu(x)$, respectively. In addition, Eq. (B10) implies that the weight function in our case is

$$w(x) = \frac{1}{\varepsilon(x)}.$$
 (B11)

Put the metric Eq. (B11) into Eq. (B9), we get the generalized orthogonal condition for two different wave functions $H_y(x)$, which is precisely Eq. (7) in the main text.

The above discussion enables us to find the appropriate metric functions in more general cases. For example, still in the TM case, if one rather chooses the E_x field as the wave functions, then it is easy to prove that the metric function should be $w(x) = \varepsilon(x)$. On the other hand, if the polarization is TE instead, then the metric functions are completely different and should be carefully restudied.

APPENDIX C: VALIDATION OF OUR THEORY UNDER OBLIQUE INCIDENCE: EFFECTS OF NONLOCAL RESPONSE

In the main text, we have verified our effective-medium theory under normal-incidence condition. Here, we further validate our theory under oblique incidences. Such a justification also proves that the nonlocal responses of the systems are not significant, so that our theory, even without considering the nonlocal effects in its present form, can still work very well.

In general, the grating structure should be considered as a uniaxial anisotropic medium with effective permittivity tensor given as

$$\vec{\varepsilon}_{\text{eff}} = \begin{pmatrix} \varepsilon_{\perp} & 0 & 0\\ 0 & \varepsilon_{\parallel} & 0\\ 0 & 0 & \varepsilon_{\parallel} \end{pmatrix}, \quad (C1)$$

where ε_{\perp} has been given by our theory. The value of ε_{\parallel} , on the hand, can also be easily obtained by extending our theory to the TE polarization (still under normal incidence), which can done by noticing the symmetries between \vec{E} and \vec{H} fields in TM and TE cases.

With ε_{eff} known from our theory, we next take two representative grating structures to validate our theory under oblique incidences. Fixing the working wavelength at $\lambda = 25d$, we employed both our theory and the FDTD method to compute the transmittance/reflectance of two grating structures (with thicknesses h = 10d) under different incidence angles. Comparison between FDTD and the effective-medium theory (Fig. 7) indicates that our theory works well under oblique incidences.

APPENDIX D: EXPERIMENTAL DETAILS

Figure 8(a) shows a picture of the AB grating sample that we fabricated and experimentally characterized. The microwave transmittance spectra were measured by a vector network analyzer (Agilent E8362C PNA) and the experimental setup is shown in Fig. 8(b). Two identical horns, separated by a distance of 106 cm and connected to the network analyzer, were used



FIG. 9. (Color online) Transmittance spectra measured with and without using the time-domain gating.

to generate and receive the microwave signals. The microwave generated from the horn is polarized with $\vec{E} || \hat{x}$, and is normally coupled into the AB grating. The sample was placed on a stage, 50 cm away from the receiving horn. The transmittance is normalized to that measured without the samples. In our experiments, we used a time-domain gating technique [36] to cut in the time domain the high-order Fabry-Perot signals,

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contributed by multiple reflections between two horns. Such a technique, widely used in literature [37,38], can help us filter out the pure transmission/reflection signals contributed by the sample alone, and thus significantly improve the precision and stability of the measurement. The transmittance spectra measured with and without using the time-domain gating are compared in Fig. 9.

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