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Closed-form expression for the scattering coefficients at an interface between two periodic media

W. Śmigaj,[1] P. Lalanne,[1,a),b)] J. Yang,[1] T. Paul,[2] C. Rockstuhl,[2] and F. Lederer[2]
[1]Laboratoire Charles Fabry de l'Institut d'Optique, CNRS, Univ Paris-Sud, Campus Polytechnique, 91127 Palaiseau Cedex, France
[2]Institute of Condensed Matter Theory and Solid State Optics, Abbe Center of Photonics, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

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We use the Bloch-mode orthogonality to derive simple closed-form expressions for the scattering coefficients at an interface between two periodic media, a computationally-challenging electromagnetic scattering problem that can be solved only with advanced numerical tools. The derivation relies on the assumptions that the interface is illuminated by the fundamental Bloch mode and that the two media have only slightly different geometrical parameters. Through comparison with fully-vectorial three-dimensional computations, the analytical expressions are shown to be highly predictive for various geometries, including dielectric waveguides and metallic metamaterials. They can thus be used with confidence for designing and engineering stacks of periodic structures. © 2011 American Institute of Physics. [doi:10.1063/1.3565970]

Due to the possibility of controlling light at the wavelength scale in the optical domain, periodic nanostructures, such as photonic crystals (PhCs) and metamaterials, have attracted a considerable deal of interest within the past decades. Scientific breakthroughs have been enabled by the significant progress of nanotechnologies, which now allows the fabrication of dielectric or metallic periodic nanostructures with feature sizes down to several tens of nanometers. Although periodicity is indeed important, many devices are not fully periodic and include either local defects or tapers with a gradient of the geometrical parameters. Understanding wave scattering at an interface of two periodic media therefore has become a major issue.

Fully-vectorial, three-dimensional (3D) calculations of the scattering coefficients of such interfaces also represent a challenging electromagnetic problem, for which very few numerical tools are presently available.[1,2] In this letter, we derive analytical expressions for the scattering coefficients between the fundamental Bloch modes (BMs) of two periodic media. Under the assumption that the media differ only weakly, we show that very simple but accurate, closed-form expressions can be derived for the scattering coefficients of the fundamental BMs. Furthermore, if we assume that the fundamental BM represents the main channel for the energy transport (single-BM approximation), the propagation in stacks of periodic media can then be handled analytically by multiplication of 2×2 transfer matrices involving those coefficients. The present derivation is motivated by the fact that simple intuitive theoretical formalisms have not been presented yet and that realistic expressions for coupling strengths at periodic interfaces may be useful for designing photonic devices, such as mode converters in periodic waveguides,[3–5] tapered PhC mirrors,[6,7] or graded index beamers,[8,9] for defining the impedance of PhCs,[10] or for the theoretical study of the impact of fabrication imperfections in slow-light PhC waveguides,[11] to quote a few of them.

Let us consider the scattering problem shown in Fig. 1, where the incident fundamental mode $|\mathbf{P}_1\rangle$ in the left periodic medium impinges on an interface separating two periodic media. We adopt a Cartesian system hereafter with axes x, y, and z, the axis z being normal to the interface. The field on both sides of the interface can be expanded into a BM basis, and using the field continuity relations at $z=0$, we have

$$|\mathbf{P}_1\rangle + r_1|\mathbf{P}_{-1}\rangle + \sum_{m>1} r_m|\mathbf{P}_{-m}\rangle = t_1|\mathbf{B}_1\rangle + \sum_{m>1} t_m|\mathbf{B}_m\rangle. \qquad (1)$$

Equation (1), which is valid for the tangential field components, defines the reflection and transmission scattering coefficients r_m and t_m. Note that, on both sides of the equation, we have isolated the predominant outgoing fundamental BMs, labeled $|\mathbf{P}_{-1}\rangle$ and $|\mathbf{B}_1\rangle$. The positive and negative subscripts refer to BMs propagating toward the positive and negative z-directions, respectively. Our goal is to derive approximate expressions for the reflection and transmission coefficients, r_1 and t_1, by relying only on the knowledge of the fundamental BMs of the periodic media, the higher-order BMs being assumed to be unknown. Because a rigorous solution of Eq. (1) with fully-vectorial software is computationally expensive, such approximate expressions are anticipated to facilitate the preliminary stages of the design of

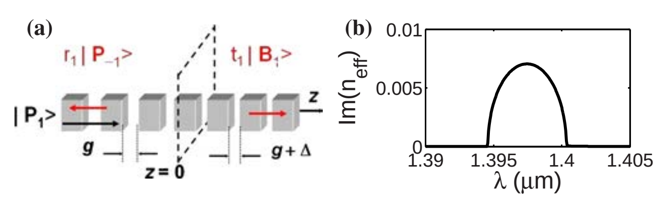

FIG. 1. (Color online) Scattering at the interface of two z-periodic media. In the transverse x- and y-directions the media can be periodic, like a fishnet, or aperiodic, like in the z-periodic GWs shown in (a). Only the fundamental BMs, $|\mathbf{P}_1\rangle$ (incident), $|\mathbf{P}_{-1}\rangle$ (reflected), and $|\mathbf{B}_1\rangle$ (transmitted), are shown. (b) Imaginary part of the effective index of $|\mathbf{P}_1\rangle$.

a)Author to whom correspondence should be addressed. Electronic mail: philippe.lalanne@institutoptique.fr.
b)Also at Laboratoire Photonique, Numériques et Nanosciences, Université Bordeaux 1, CNRS, Institut d'Optique, 33405 Talence Cedex, France.

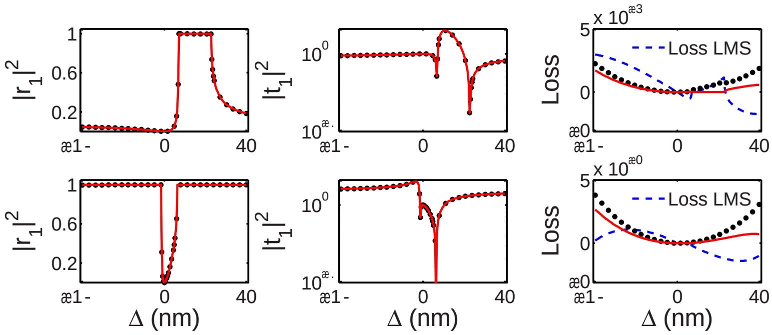

FIG. 2. (Color online) Test of closed form expressions for an interface between two subwavelength GWs. Red curves: Predictions of Eqs. (4) and (5). Black dots: fully-vectorial calculations obtained with the a-FMM by solving Eq. (1). The blue curves in the right panel represent the out-of-plane losses calculated by solving Eq. (2) in the LMS sense. (a) $\lambda=1.41$ μm, (the incident BM $|\mathbf{P}_1\rangle$ is a propagating BM). (b) $\lambda=1.398$ μm ($|\mathbf{P}_1\rangle$ is a gap evanescent BM).

complicated components involving stacks of periodic structures.

It is first tempting to neglect all the unknown quantities,[10,12,13] i.e., the higher-order BMs, to end up with a simplified version of Eq. (1) that reads as

$$|\mathbf{P}_1\rangle + r_1|\mathbf{P}_{-1}\rangle = t_1|\mathbf{B}_1\rangle. \tag{2}$$

Assuming that $|\mathbf{P}_1\rangle,|\mathbf{P}_{-1}\rangle$ and $|\mathbf{B}_1\rangle$, are known at $z=0$, the coefficients r_1 and t_1 can be obtained by projecting Eq. (2) on a complete set of functions $|\mathbf{F}_n\rangle$—for instance Fourier harmonics—and solving the resulting system of equations in the least-mean-squares (LMS) sense. As will be shown, however, the accuracy of the LMS solution is poor. This is because Eq. (2) authoritatively states an over-simplified expression for the fields on *both* sides of the interface and completely ignores the role of higher-order BMs involved in the coupling mechanism. Actually, it is possible to take them into account, at least approximately, without explicitly calculating them, and one may derive analytical expressions for r_1 and t_1 that are more accurate than those obtained with the LMS approach. This is at the heart of this letter. The elimination of the unknown higher-order BMs in Eq. (1) can be achieved, under the sole assumption that the materials are reciprocal, by using BM orthogonality, which reads[1]

$$\langle \mathbf{B}_n|\mathbf{B}_m\rangle = \int\int_S [\mathbf{E}_m \times \mathbf{H}_n - \mathbf{E}_n \times \mathbf{H}_m] \cdot \mathbf{z} dS = 0 \quad \text{if } m \neq -n. \tag{3}$$

In Eq. (3), $|\mathbf{B}_n\rangle$ and $|\mathbf{B}_m\rangle$ are two BMs of the same periodic medium, S represents an (x,y) cross-section of the medium, and $\mathbf{E}_n$ and $\mathbf{H}_n$ are the electric and magnetic transverse components of $|\mathbf{B}_n\rangle$, $\mathbf{z}$ being the unit vector normal to the interface. Equation (3) defines an antisymmetric bilinear form: $\langle \mathbf{B}_m|\mathbf{B}_n\rangle = -\langle \mathbf{B}_n|\mathbf{B}_m\rangle$. Hereafter, the BMs are normalized so that $\langle \mathbf{B}_n|\mathbf{B}_{-n}\rangle=4$, implying that nonevanescent truly guided BMs propagating in lossless periodic media have unit power flow along the z axis.[1]

Coming back to Eq. (1), we start by deriving an approximate closed-form expression for r_1. Under the assumption that the two periodic media are only slightly different, it is expected that the scattering process predominantly consists in exciting the fundamental BMs, $|\mathbf{P}_{-1}\rangle$ and $|\mathbf{B}_1\rangle$, the excitation of the higher-order BMs being a weaker process induced by the transverse mode-profile mismatch between the fundamental BMs $|\mathbf{P}_1\rangle$ and $|\mathbf{B}_1\rangle$.[14] Therefore, an accurate expression for the reflection coefficient r_1 can be derived by neglecting the high-order transmitted BMs, and we obtain $|\mathbf{P}_1\rangle + r_1|\mathbf{P}_{-1}\rangle + \Sigma_{m>1} r_m|\mathbf{P}_{-m}\rangle \approx t_1|\mathbf{B}_1\rangle$. Then, without any further approximation, we use the BM orthogonality and project the previous equation onto $\langle \mathbf{P}_1|$ and $\langle \mathbf{P}_{-1}|$, to get $r_1\langle \mathbf{P}_1|\mathbf{P}_{-1}\rangle = t_1\langle \mathbf{P}_1|\mathbf{B}_1\rangle$ and $\langle \mathbf{P}_{-1}|\mathbf{P}_1\rangle = t_1\langle \mathbf{P}_{-1}|\mathbf{B}_1\rangle$, from which we eliminate t_1 to obtain

$$r_1 = -\langle \mathbf{P}_1|\mathbf{B}_1\rangle / \langle \mathbf{P}_{-1}|\mathbf{B}_1\rangle. \tag{4}$$

Consistently, to calculate t_1, we first neglect the high-order reflected BMs and, after projecting onto $\langle \mathbf{B}_1|$ and $\langle \mathbf{B}_{-1}|$, we obtain $r_1\langle \mathbf{B}_{-1}|\mathbf{P}_{-1}\rangle + \langle \mathbf{B}_{-1}|\mathbf{P}_1\rangle = t_1\langle \mathbf{B}_{-1}|\mathbf{B}_1\rangle$ and $\langle \mathbf{B}_1|\mathbf{P}_1\rangle + r_1\langle \mathbf{B}_1|\mathbf{P}_{-1}\rangle = 0$. The elimination of r_1 leads to

$$4t_1 = \langle \mathbf{B}_{-1}|\mathbf{P}_1\rangle - \langle \mathbf{B}_{-1}|\mathbf{P}_{-1}\rangle\langle \mathbf{B}_1|\mathbf{P}_1\rangle / \langle \mathbf{B}_1|\mathbf{P}_{-1}\rangle. \tag{5}$$

The closed-form expressions of Eqs. (4) and (5) constitute the main result of the present work. Henceforth, their accuracy will be tested for various geometries, such as metallic metamaterials and dielectric waveguides.

Let us first consider an interface [Fig. 1(a)] between two sub-λ grating waveguides (GWs). Every GW is a composite medium formed by periodically interlacing Si ($n=3.48$) segments embedded in a SiO_2 ($n=1.44$) host medium. Remarkably low propagation loss of 2.1 dB/cm in the telecom C-band has been recently reported[15] for this geometry. The segment dimensions of the GW on the left side of the interface are $c_x=300$ nm, $c_y=260$ nm, and $c_z=300$ nm, and the grating period is $a_z=400$ nm corresponding to a SiO_2 gap length $g=100$ nm. We have calculated the band structure of the fundamental TE-like BM (with $E_y=0$ on $y=0$) with the aperiodic Fourier modal method (a-FMM).[1] The BM is truly guided in the spectral range of interest. Figure 1(b) shows the imaginary part of its effective index n_{eff}, i.e., its normalized wave vector. Note that, for 1.394 μm $<\lambda<$ 1.404 μm, a band gap opens and $\text{Im}(n_{\text{eff}})$ is positive: the fundamental BM is evanescent. The GW on the right-hand side of the interface [see Fig. 1(a)] has similar dimensions, except that the SiO_2 gap width is augmented by an incremental value Δ subject to variations.

We have computed the scattering coefficients at the interface with the a-FMM. We first determine the complete set of BMs in the two media by diagonalizing the scattering matrix relating the field amplitudes in two planes separated by a_z. In a second step, we expand the field in each periodic medium in a BM basis, and by using Fourier-series expansions to match the tangential field components at the interface, we compute the scattering coefficients of all BMs, i.e., all the r_m and t_m in Eq. (1). Figure 2 compares the scattering coefficients, $|r_1|^2$ and $|t_1|^2$, obtained with the a-FMM (black dots) and with Eqs. (4) and (5) (red curves). The upper plots in Fig. 2(a) are obtained for $\lambda=1.41$ μm; $|\mathbf{P}_1\rangle$ is propagating and $|\mathbf{B}_1\rangle$ can be either propagating or evanescent. For the lower curves, $\lambda=1.398$ μm, the incident BM is evanescent, and in the spectral region where $|r_1|^2$ is significantly smaller

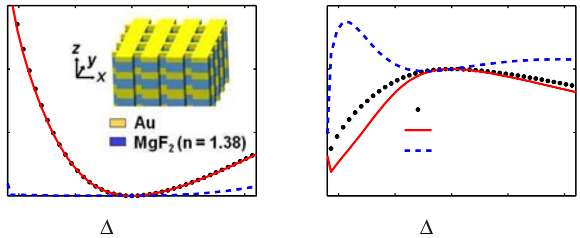

FIG. 3. (Color online) Test of closed-form expressions for an interface between two fishnets. (a) $|r_1|^2$. (b) $|t_1|^2$. The fishnet parameters are those in Ref. 16: the periodicity in the x- and y-directions is $a_x=a_y=860$ nm, the rectangular hole dimensions are $w_x=295$ nm and $w_y=595$ nm. The refractive index of MgF_2 is 1.38 and the gold permittivity is $-142+18.7i$ at $\lambda=1.9$ μm. The calculation is performed for BMs with $H_y(x)=H_y(-x)$. The inset sketches the fishnet geometry.

than one, $|\mathbf{B}_1\rangle$ is evanescent too. We note that an excellent agreement is achieved for all plots; for instance in Fig. 2(b), the maximum deviation between the a-FMM data and the approximate expressions is only 0.009 and 0.004 for $|t_1|^2$ and $|r_1|^2$, respectively. The right panel shows the out-of-plane losses L at the interface for an incident BM normalized so that $\langle \mathbf{P}_1 | \mathbf{P}_{-1}\rangle=4$. L can be simply calculated as the difference between the longitudinal (along z) power flow of $|\mathbf{P}_1\rangle+r_1|\mathbf{P}_{-1}\rangle$ and that of $t_1|\mathbf{B}_1\rangle$. Note that when both $|\mathbf{P}_1\rangle$ and $|\mathbf{P}_{-1}\rangle$ are evanescent like in Fig. 2(b), the standing evanescent field, $|\mathbf{P}_1\rangle+r_1|\mathbf{P}_{-1}\rangle$, carries some net power flow, although the power flow of every individual BM is null. It is worth emphasizing that the loss predictions obtained with the closed-form expressions of Eqs. (4) and (5) are much more accurate than those obtained by calculating r_1 and t_1 with Eq. (2) with the LMS approach (blue curves). Additionally note that the loss LMS values are inconsistently found to be negative for some values of Δ.

The accuracy of Eqs. (4) and (5) has also been tested for completely different structures, by considering an interface between two fishnets. The reference fishnet consists of an array of rectangular air-holes etched in an Au(15 nm)–MgF_2(50 nm)–Au(15 nm) periodic stack [see inset in Fig. 3(a)], with the parameters reported in Ref. 16 (see details in the caption of Fig. 3). This important geometry has been thoroughly analyzed in Ref. 17, where the authors have shown that the energy transfer through the fishnet is predominantly due to a single BM. The second fishnet is identical to the reference one, except that the MgF_2-layer thickness is increased by Δ. Figure 3 compares the scattering coefficients, $|r_1|^2$ and $|t_1|^2$, obtained with the a-FMM (black dots) and with Eqs. (4) and (5) (red curves). The computation is performed for a normally-incident BM (Ref. 18) and $\lambda=1.9$ μm, corresponding to a negative effective index $n_{\mathrm{eff}}=-2.93+0.34i$. Again the predictions obtained with Eqs. (4) and (5) are quantitative and much more accurate than those obtained with the LMS approach (blue curves), which are completely erroneous except for $|\Delta|<5$ nm. Indeed, the fishnet problem represents a challenging test, much more difficult than the GW geometry, for which the fundamental BM is essentially a superposition of two counter-propagating fundamental guided modes of the silicon ridges.[14] For the fishnet, a 30 nm incremental value represents a substantial perturbation (remember that the reference dielectric thickness is 50 nm), and because the thickness of the metallic layer (30 nm) is comparable to the skin depth, several BMs are excited at the interface. This explains why the LMS approach completely fails for incremental values larger than a few nanometers.

The accuracy improvement brought about by the BM-orthogonality approach can be understood as follows. For small increments Δ, the overlap integrals $\langle \mathbf{P}_n | \mathbf{B}_m\rangle$ are $O(\Delta)$ for $n\neq \pm m$ and the higher-order coefficients r_m and t_m are also $O(\Delta)$ for $m>1$. Therefore, by neglecting the terms $r_m\langle \mathbf{B}_{\pm 1} | \mathbf{P}_{-m}\rangle$ and $t_m\langle \mathbf{P}_{\pm 1} | \mathbf{B}_m\rangle$ $(m>1)$ in the derivation of Eqs. (4) and (5) one commits an error of only $O(\Delta^2)$. In contrast, when we solve Eq. (2) in the LMS sense, the terms $r_m\langle \mathbf{F}_n | \mathbf{P}_{-m}\rangle$ and $t_m\langle \mathbf{F}_n | \mathbf{B}_m\rangle$ $(m>1)$ are neglected and, since the coefficients $\langle \mathbf{F}_n | \mathbf{P}_{-m}\rangle$ and $\langle \mathbf{F}_n | \mathbf{B}_m\rangle$ are $O(1)$ in general, the error is of the order $O(\Delta)$.

We conclude that simple and accurate closed-form expressions for the scattering at an interface between two slightly different periodic media can be derived using BM orthogonality, even if one assumes that only the fundamental BMs of the two media are known. The accuracy of the expressions have been thoroughly tested for several distinct geometries, including purely dielectric periodic waveguides offering large variations of the scattering coefficients in the vicinity of the band edges and metallodielectric structures providing rapid changes in the BM profiles as one slightly tunes the geometrical parameters. High accuracy has been obtained in all cases, letting us expect that the expressions are reliable and can be used with confidence to design graded periodic structures.

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[1] G. Lecamp, J. P. Hugonin, and P. Lalanne, Opt. Express **15**, 11042 (2007).
[2] A. Fallahi and C. Hafner, J. Opt. Soc. Am. A **27**, 40 (2010).
[3] T. Z. Weissman and A. Hardy, Electron. Lett. **28**, 1514 (1992).
[4] P. Lalanne and A. Talneau, Opt. Express **10**, 354 (2002).
[5] A. O. Cakmak, E. Colak, H. Caglayan, H. Kurt, and E. Ozbay, J. Appl. Phys. **105**, 103708 (2009).
[6] P. Lalanne, C. Sauvan, and J. P. Hugonin, Laser Photonics Rev. **2**, 514 (2008).
[7] A. R. Md Zain, N. P. Johnson, M. Sorel, and R. M. De La Rue, Opt. Express **16**, 12084 (2008).
[8] E. Centeno and D. Cassagne, Opt. Lett. **30**, 2278 (2005).
[9] H. Kurt and D. S. Citrin, Opt. Express **15**, 1240 (2007).
[10] W. Śmigaj and B. Gralak, Phys. Rev. B **77**, 235445 (2008).
[11] S. Mazoyer, J. P. Hugonin, and P. Lalanne, Phys. Rev. Lett. **103**, 063903 (2009).
[12] B. Momeni, A. A. Eftekhar, and A. Adibi, Opt. Lett. **32**, 778 (2007).
[13] R. Biswas, Z. Y. Li, and K. M. Ho, Appl. Phys. Lett. **84**, 1254 (2004).
[14] M. Palamaru and P. Lalanne, Appl. Phys. Lett. **78**, 1466 (2001).
[15] P. J. Bock, P. Cheben, J. H. Schmid, J. Lapointe, A. Delâge, S. Janz, G. C. Aers, D. X. Xu, A. Densmore, and T. J. Hall, Opt. Express **18**, 20251 (2010).
[16] J. Valentine, S. Zhang, T. Zentgraf, E. Ulin-Avila, D. Genov, G. Bartal, and X. Zhang, Nature (London) **455**, 376 (2008).
[17] J. Yang, C. Sauvan, T. Paul, C. Rockstuhl, F. Lederer, and P. Lalanne, Appl. Phys. Lett. **97**, 061102 (2010).
[18] For oblique incidence fixed by the in-plane Bloch-wave vector $[k_x,k_y]\neq 0$, the orthogonality relation of Eq. (3) must be modified to involve modes $|\mathbf{B}_n\rangle$ and $|\mathbf{B}_m\rangle$ with opposite in-plane Bloch-wave vectors $[k_x,k_y]$ and $[-k_x,-k_y]$, respectively.